

Correlation functions of the open XXZ chain I

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Abstract

We consider the XXZ spin chain with diagonal boundary conditions in the framework of algebraic Bethe Ansatz. Using the explicit computation of the scalar products of Bethe states and a revisited version of the bulk inverse problem, we calculate the elementary building blocks for the correlation functions. In the limit of half-infinite chain, they are obtained as multiple integrals of usual functions, similar to the case of periodic boundary conditions.

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1 Introduction

Doped low-dimensional antiferromagnets have attracted a lot of studies especially since the discovery of high-Tc superconductivity. A particularly simple form of doping results from replacing some magnetic ions of the crystal by nonmagnetic one's. Open Heisenberg quantum spin chains [1] are the archetype of one-dimensional models providing microscopic description of such systems. Indeed, the presence of non-magnetic impurities into crystals having effective one-dimensional magnetic behavior has drastic effects on their low energy properties : the chain is cut into finite pieces with essentially free (open) boundaries leading to the breaking of translational invariance. As a consequence, physical quantities such as for example the magnetic susceptibility will get measurable corrections due to the presence of the boundary [2–11]. The same quantum spin chains have also acquired recently an important role in the study and the understanding of the interplay between quantum entanglement and quantum criticality [12–20]. There, the presence of boundaries also leads to noticeable effects, like in particular Friedel oscillations [21–23] and the algebraic decrease of the boundary part of the entanglement entropy as a function of the distance to the boundary [19, 20].

Correlation functions are central in the description of such effects and are in fact accessible in experiments. In particular the local magnetic susceptibility in the presence of boundary can be obtained using muon spin rotation/relaxation on the corresponding crystals, see for example [11]. More generally, correlation functions contain the necessary information to compare the microscopic models at hand to the reality, in particular through the measurements of dynamical structure factors accessible by neutron scattering experiments [24–30]. While the computation of exact spectrum of Heisenberg chains has already a very long history, see e.g. [31–44], and references therein, computation of exact correlation functions of integrable lattice models such as Heisenberg spin chains, in particular out of their free fermion point where already considerable work was necessary [45–53], has been a major challenge for the last twenty years. Progress have been obtained using different routes and several results are now available for the correlation in the bulk, i.e., far from the boundaries [41, 42, 54–81], although still more progress is needed to obtain full answers. Advances have been obtained also in the presence of a boundary using in particular q -vertex operator methods [82, 83] and field theory approach [6–10, 84–92].

The aim of the present paper is to develop a method to compute correlation functions of integrable open (finite and semi-infinite) spin chains in the framework of the (algebraic) Bethe ansatz for boundary integrable models [93–105]. For this purpose, we will consider the example of the finite XXZ spin-1/2 Heisenberg chain with diagonal boundary conditions, including in particular non-zero boundary longitudinal magnetic fields, and its (semi-infinite) thermodynamic limit. Our results concern the general elementary blocks of correlation functions at zero temperature, namely the average value of arbitrary products spin operators going from the boundary to an arbitrary site at distance m from this boundary. Any correlation function can be written in terms of these

elementary blocks. Previous attempts towards this goal in the Bethe ansatz framework can be found in [7, 106–108].

The strategy we will follow to solve this problem is closely related to the one used in the periodic case [59, 60]. The central object in this approach is provided by the monodromy matrix of the open chain, which is a function of a complex spectral parameter λ and of inhomogeneous parameters ξ_i attached to each site of the chain. Following Sklyanin [95], it is given as a quadratic expression in terms of the standard (bulk) monodromy matrix with the adjunction of the so called boundary K -matrix which encode the boundary conditions [95, 96, 100]; in this paper only diagonal K -matrices will be considered. This boundary monodromy matrix satisfies a boundary Yang-Baxter algebra governed by two R -matrices while the K -matrix itself satisfies its c-number version also called reflection equation [95]. These settings have been used by Sklyanin to extend the algebraic Bethe ansatz method to this open case. In particular, the Hamiltonian of the chain can then be reconstructed in terms of a weighted (with the K matrix) trace of this monodromy matrix. Hence as in the periodic case, one can consider a common set of eigenstates of the boundary transfer matrix and of the Hamiltonian.

The first task towards the computation of the correlation functions is to identify the space of states of the open chain as generated by the action of the entries of the boundary monodromy matrix (depending on different spectral parameters λ_j) on some reference state (here the state with all spins up or down); then eigenstates of the open chain are obtained from such actions thanks to the Bethe ansatz equations for the spectral parameters λ_j [94, 95]. Using this framework, we will show that it is possible to find determinant expressions for the scalar product between a boundary Bethe state and an arbitrary boundary state and consequently for the norm of the Bethe eigenstates. This is achieved along the lines used for the bulk case in [59] using the factorizing F -matrix basis [58].

The second problem is to obtain the action of the local spin operators on such states. In the bulk case, it was given by the resolution of the quantum inverse scattering problem, namely, by the reconstruction of such local operators in site j in terms of a simple monodromy matrix elements (evaluated at $\lambda = \xi_j$) multiplied from the right and from the left by products of the transfer matrices evaluated in the inhomogeneity parameters ξ_i for $i = 1, \dots, j$. In this bulk case, the Bethe eigenstates of the Heisenberg chain Hamiltonian being also common eigenstates for the transfer matrix, it was straightforward to obtain the explicit action of the local spin operators on such Bethe states.

The situation in the presence of boundaries turns out to be slightly more subtle : due to the breaking of translation invariance, boundary Bethe states are no longer eigenstates of the bulk transfer matrix, hence leading to a difficult combinatorial problem while using the expression of local operators described above.

We solve this problem in three steps :

- (i) We first find a general (simple) relation relating boundary Bethe states to bulk one's.
- (ii) Then the reconstruction of local spin operators is obtained through a rewriting of the above quantum inverse scattering problem solution as a unique monomial in terms of the bulk monodromy matrix entries, avoiding in particular the presence of products of transfer matrices; it gives a new form for the general solution of the quantum inverse

scattering problem.

(iii) Due to this new form of the solution of the quantum inverse scattering problem, the action of the local spin operators on any boundary Bethe state (expressed in terms of bulk one's) can then be given in a simple way and the result can be rewritten back in terms of sums of boundary Bethe states.

Then, using scalar product and norm formulas for boundary states, we obtain any correlation functions as explicit sums of ratio of determinants of size half the length of the chain. In the thermodynamic limit (the limit of semi-infinite chain), these sums become multiple integrals with weights given in terms of the density of Bethe roots in the boundary ground state; this density function indeed describes the infinite size limit of the above ratios of determinants. For the so-called elementary blocks of correlation functions it gives proofs of the multiple integrals representations obtained previously [82,83] using the q -vertex operator method, here both in the massive and massless regimes of the chain. The problem of computing physical spin correlation functions will be addressed in a subsequent paper; this involves summing large number of the elementary blocks obtained here, using techniques similar to the one's developed for the bulk case [62,63].

This paper is organized as follows. In Section 2, we briefly describe the open XXZ chain with integrable diagonal boundary conditions and introduce the main notations. Section 3 contains some elementary algebraic properties of boundary operators and boundary states, and a description of the ground state in the thermodynamic limit. In Section 4, the scalar products of Bethe eigenstates with arbitrary dual states are computed. In Section 5, we explain how, using a new version of the bulk inverse problem, one can derive the action of a product of elementary matrices on a boundary arbitrary state. Finally, in Section 6, elementary building blocks of the correlation functions are computed using the results of Section 5 and Section 4, and we give their multiple integral representation in the thermodynamic limit. Some technical details are gathered in a set of appendices.

2 The boundary XXZ chain: definitions and notations

In this paper, we consider the XXZ Heisenberg spin-1/2 finite chain with diagonal boundary conditions. The Hamiltonian of a chain of M sites is given by

$$\mathcal{H} = \sum_{m=1}^{M-1} \left\{ \sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y + \Delta (\sigma_m^z \sigma_{m+1}^z - 1) \right\} + h_- \sigma_1^z + h_+ \sigma_M^z. \quad (2.1)$$

The local spin operators σ_m^x , σ_m^y and σ_m^z at site m act as the corresponding Pauli matrices in the local quantum space $\mathcal{H}_m \sim \mathbb{C}^2$, and as the identity operator elsewhere. The quantum space of states of the chain is $\mathcal{H} = \otimes_{m=1}^M \mathcal{H}_m$. In (2.1), Δ is the bulk anisotropy parameter, and h_{\pm} denote the boundary fields. In what follows, they will be parametrized as $\Delta = \cosh \eta$ and $h_{\pm} = \sinh \eta \coth \xi_{\pm}$.

To diagonalize the boundary Hamiltonian \mathcal{H} , we use the modified version of the algebraic Bethe Ansatz proposed by Sklyanin in [95]. As in the case of periodic boundary

conditions, the eigenvectors are obtained as those of a family of commuting transfer matrices, which are constructed as follows.

Let $R : \mathbb{C} \rightarrow \text{End}(V \otimes V)$, $V \sim \mathbb{C}^2$, denote the R -matrix of the XXZ model,

$$R(u) = \sinh(u + \eta) \hat{R}(u), \quad \text{with} \quad \hat{R}(u) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(u) & c(u) & 0 \\ 0 & c(u) & b(u) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (2.2)$$

in which

$$b(u) = \frac{\sinh u}{\sinh(u + \eta)}, \quad c(u) = \frac{\sinh \eta}{\sinh(u + \eta)}. \quad (2.3)$$

It is obtained as the trigonometric solution of the Yang-Baxter equation¹,

$$R_{12}(u - v) R_{13}(u - w) R_{23}(v - w) = R_{23}(v - w) R_{13}(u - w) R_{12}(u - v). \quad (2.4)$$

The R -matrix satisfies the following initial, unitarity and crossing symmetry relations:

$$\hat{R}(0) = \mathcal{P}, \quad (2.5)$$

$$\hat{R}_{12}(u) \hat{R}_{21}(-u) = 1, \quad (2.6)$$

$$\sigma_1^y R_{12}^{t_1}(u - \eta) \sigma_1^y = -R_{21}(-u). \quad (2.7)$$

Here \mathcal{P} is the permutation operator on $V \otimes V$, $R_{21} = \mathcal{P}_{12} R_{12} \mathcal{P}_{12}$, and t_1 denotes the matrix transposition on the first space of the tensor product.

Let also $K(u; \xi)$ be the boundary matrix

$$K(u) = K(u; \xi) = \begin{pmatrix} \sinh(u + \xi) & 0 \\ 0 & \sinh(\xi - u) \end{pmatrix}, \quad (2.8)$$

corresponding to the diagonal solution of the boundary Yang-Baxter equation [96]

$$R_{12}(u - v) K_1(u) R_{12}(u + v) K_2(v) = K_2(v) R_{12}(u + v) K_1(u) R_{12}(u - v). \quad (2.9)$$

A commuting family of transfer matrices $\mathcal{T}(\lambda) \in \text{End } \mathcal{H}$ is constructed from R and K as

$$\mathcal{T}(\lambda) = \text{tr}_0 \{ K_+(\lambda) T(\lambda) K_-(\lambda) \hat{T}(\lambda) \}. \quad (2.10)$$

Here the trace is taken over an auxiliary space $V_0 \sim \mathbb{C}^2$, $K_{\pm}(\lambda) = K(u \pm \eta/2; \xi_{\pm}) \in \text{End } V_0$, $T(\lambda) \in \text{End}(V_0 \otimes \mathcal{H})$ is the bulk monodromy matrix,

$$T(\lambda) = R_{0M}(\lambda - \xi_M) \dots R_{02}(\lambda - \xi_2) R_{01}(\lambda - \xi_1), \quad (2.11)$$

¹Here and in the following, indices label the spaces of the tensor product in which the corresponding operator acts non trivially. For example, in (2.4), which is an equation on $V_1 \otimes V_2 \otimes V_3$, $V_i \sim \mathbb{C}^2$, R_{ij} denotes the R -matrix (2.2) acting in $V_i \otimes V_j$.

and $\widehat{T}(\lambda)$ is defined as

$$\widehat{T}(\lambda) = R_{10}(\lambda + \xi_1 - \eta) R_{20}(\lambda + \xi_2 - \eta) \dots R_{M0}(\lambda + \xi_M - \eta). \quad (2.12)$$

In these last expressions, R_{0m} denotes the R -matrix in $\text{End}(V_0 \otimes \mathcal{H}_m)$, and $\xi_1, \xi_2, \dots, \xi_M$ are arbitrary complex parameters (inhomogeneity parameters) attached to the different sites of the chain. Note that, due to (2.6) and (2.7),

$$\widehat{T}(\lambda) = \gamma(\lambda) \sigma_0^y T^{t_0}(-\lambda) \sigma_0^y \quad (2.13)$$

$$= \widehat{\gamma}(\lambda) T^{-1}(-\lambda + \eta), \quad (2.14)$$

with, in our normalization,

$$\gamma(\lambda) = (-1)^M, \quad \widehat{\gamma}(\lambda) = (-1)^M \prod_{j=1}^M [\sinh(\lambda + \xi_j) \sinh(\lambda + \xi_j - 2\eta)]. \quad (2.15)$$

In the homogeneous limit ($\xi_m = \eta/2$ for $m = 1, \dots, M$), the Hamiltonian (2.1) can be obtained as the following derivative of the transfer matrix (2.10):

$$\mathcal{H} = \frac{2 [\sinh \eta]^{1-2M}}{\text{tr}\{K_+(\eta/2)\} \text{tr}\{K_-(\eta/2)\}} \frac{d}{d\lambda} \mathcal{T}(\lambda) \Big|_{\lambda=\eta/2} + \text{constant}. \quad (2.16)$$

In the case of periodic boundary conditions, the space of states is constructed in terms of the operator entries $A, B, C, D \in \text{End} \mathcal{H}$ of the bulk monodromy matrix (2.11) expressed as a 2×2 matrix acting on the auxiliary space:

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}. \quad (2.17)$$

These operators satisfy a quadratic algebra given by the following quadratic relation on $V_1 \otimes V_2 \otimes \mathcal{H}$, $V_i \sim \mathbb{C}^2$:

$$R_{12}(\lambda - \mu) T_1(\lambda) T_2(\mu) = T_2(\mu) T_1(\lambda) R_{12}(\lambda - \mu). \quad (2.18)$$

In this framework, eigenstates of the periodic Hamiltonian are constructed as the multiple action of creation operators $B(\lambda_j)$ on the reference state $|0\rangle$ with all spins up, provided that the corresponding spectral parameters λ_j satisfy the bulk Bethe equations.

In the case of the diagonal boundary conditions (2.1), a similar construction can be performed (see [95]) using the operators entries $\mathcal{A}_-, \mathcal{B}_-, \mathcal{C}_-, \mathcal{D}_- \in \text{End} \mathcal{H}$ (respectively $\mathcal{A}_+, \mathcal{B}_+, \mathcal{C}_+, \mathcal{D}_+$) of one of the “double-row” monodromy matrices \mathcal{U}_- or \mathcal{U}_+ defined on $\text{End}(V_0 \otimes \mathcal{H})$ as

$$\mathcal{U}_-(\lambda) = T(\lambda) K_-(\lambda) \widehat{T}(\lambda) = \begin{pmatrix} \mathcal{A}_-(\lambda) & \mathcal{B}_-(\lambda) \\ \mathcal{C}_-(\lambda) & \mathcal{D}_-(\lambda) \end{pmatrix}, \quad (2.19)$$

$$\mathcal{U}_+^{t_0}(\lambda) = T^{t_0}(\lambda) K_+^{t_0}(\lambda) \widehat{T}^{t_0}(\lambda) = \begin{pmatrix} \mathcal{A}_+(\lambda) & \mathcal{C}_+(\lambda) \\ \mathcal{B}_+(\lambda) & \mathcal{D}_+(\lambda) \end{pmatrix}. \quad (2.20)$$

Note that the matrix \mathcal{U}_- (respectively \mathcal{U}_+), as well as its operator entries $\mathcal{A}_-, \mathcal{B}_-, \mathcal{C}_-$ and \mathcal{D}_- (respectively $\mathcal{A}_+, \mathcal{B}_+, \mathcal{C}_+$ and \mathcal{D}_+) depend also on the parameters ξ_1, \dots, ξ_M and ξ_- (respectively ξ_1, \dots, ξ_M and ξ_+). It will be sometimes necessary in the paper to specify explicitly this dependency, denoting e.g. $\mathcal{U}_-(\lambda; \xi_-)$ instead of $\mathcal{U}_-(\lambda)$. The matrices \mathcal{U}_- and \mathcal{U}_+ satisfy the boundary Yang-Baxter equations

$$\begin{aligned} R_{12}(u-v) (\mathcal{U}_-)_1(u) R_{12}(u+v-\eta) (\mathcal{U}_-)_2(v) \\ = (\mathcal{U}_-)_2(v) R_{12}(u+v-\eta) (\mathcal{U}_-)_1(u) R_{12}(u-v), \end{aligned} \quad (2.21)$$

$$\begin{aligned} R_{12}(-u+v) (\mathcal{U}_+)_1^{t_1}(u) R_{12}(-u-v-\eta) (\mathcal{U}_+)_2^{t_2}(v) \\ = (\mathcal{U}_+)_2^{t_2}(v) R_{12}(-u-v-\eta) (\mathcal{U}_+)_1^{t_1}(u) R_{12}(-u+v), \end{aligned} \quad (2.22)$$

which leads to commutation relations for their operator entries.

Note that the transfer matrices (2.10) can be expressed either in terms of the matrix elements of \mathcal{U}_- ,

$$\begin{aligned} \mathcal{T}(\lambda) &= \text{tr}_0\{K_+(\lambda)\mathcal{U}_-(\lambda)\} \\ &= \sinh(\lambda + \eta/2 + \xi_+) \mathcal{A}_-(\lambda) - \sinh(\lambda + \eta/2 - \xi_+) \mathcal{D}_-(\lambda), \end{aligned} \quad (2.23)$$

or in terms of the matrix elements of \mathcal{U}_+ ,

$$\begin{aligned} \mathcal{T}(\lambda) &= \text{tr}_0\{K_-(\lambda)\mathcal{U}_+(\lambda)\} \\ &= \sinh(\lambda - \eta/2 + \xi_-) \mathcal{A}_+(\lambda) - \sinh(\lambda - \eta/2 - \xi_-) \mathcal{D}_+(\lambda), \end{aligned} \quad (2.24)$$

and their common eigenstates can be constructed either in the form

$$|\psi_-(\{\lambda\})\rangle = \prod_{k=1}^N \mathcal{B}_-(\lambda_k) |0\rangle, \quad \langle\psi_-(\{\lambda\})| = \langle 0| \prod_{k=1}^N \mathcal{C}_-(\lambda_k), \quad (2.25)$$

or in the form

$$|\psi_+(\{\lambda\})\rangle = \prod_{k=1}^N \mathcal{B}_+(\lambda_k) |0\rangle, \quad \langle\psi_+(\{\lambda\})| = \langle 0| \prod_{k=1}^N \mathcal{C}_+(\lambda_k), \quad (2.26)$$

provided the set of spectral parameters $\{\lambda\}$ satisfies the Bethe equations

$$y_j(\lambda_j; \{\lambda\}; \xi_+, \xi_-) = y_j(-\lambda_j; \{\lambda\}; \xi_+, \xi_-), \quad j = 1, \dots, N, \quad (2.27)$$

with

$$y_j(\mu; \{\lambda\}; \xi_+, \xi_-) = \frac{\hat{y}(\mu; \{\lambda\}; \xi_+, \xi_-)}{\sinh(\lambda_j - \mu + \eta) \sinh(\lambda_j + \mu - \eta)}, \quad (2.28)$$

$$\begin{aligned} \hat{y}(\mu; \{\lambda\}; \xi_+, \xi_-) &= -a(\mu) d(-\mu) \sinh(\mu + \xi_+ - \eta/2) \sinh(\mu + \xi_- - \eta/2) \\ &\quad \times \prod_{k=1}^N [\sinh(\mu - \lambda_k - \eta) \sinh(\mu + \lambda_k - \eta)]. \end{aligned} \quad (2.29)$$

Here $a(\lambda)$ and $d(\lambda)$ stand respectively for the eigenvalue of the bulk operators $A(\lambda)$ and $D(\lambda)$ on the reference state $|0\rangle$,

$$a(\lambda) = \prod_{i=1}^M \sinh(\lambda - \xi_i + \eta), \quad d(\lambda) = \prod_{i=1}^M \sinh(\lambda - \xi_i). \quad (2.30)$$

The corresponding eigenvalue of the transfer matrix $\mathcal{T}(\mu)$ on an eigenstate (2.25) or (2.26) is

$$\begin{aligned} \tau(\mu, \{\lambda_j\}) = \gamma(\mu) & \left\{ a(\mu) d(-\mu) \frac{\sinh(2\mu + \eta) \sinh(\mu + \xi_+ - \eta/2) \sinh(\mu + \xi_- - \eta/2)}{\sinh(2\mu) \prod_{i=1}^N [b(\lambda_i - \mu) b(-\mu - \lambda_i)]} \right. \\ & \left. + a(-\mu) d(\mu) \frac{\sinh(2\mu - \eta) \sinh(\mu - \xi_+ + \eta/2) \sinh(\mu - \xi_- + \eta/2)}{\sinh(2\mu) \prod_{i=1}^N [b(\mu + \lambda_i) b(\mu - \lambda_i)]} \right\}. \end{aligned} \quad (2.31)$$

Let us finally introduce some convenient notations that we will use all along the paper: for any set of complex variables $\{x_j\}$, we define

$$x_{jk} = x_j - x_k \quad \text{and} \quad \bar{x}_{jk} = x_j + x_k. \quad (2.32)$$

3 Boundary states

3.1 Algebraic elementary properties

In this subsection, we collect some usefull elementary properties concerning boundary operators and boundary states. They mainly follow from the description of the boundary XXZ model in terms of the bulk one. Indeed, the “double-row” monodromy matrices \mathcal{U}_{\pm} of the boundary XXZ model being quadratic in terms of the bulk monodromy matrix T (see definitions (2.19)-(2.20) and formula (2.13)), the boundary operators are themselves quadratic in terms of the bulk operators.

This quadratic nature influences non-trivially the dependence on the spectral parameter of the boundary operators; in particular, a “ \mathbb{Z}_2 invariance” arises in the spectral parameter dependence of the operators \mathcal{B}_{\pm} and \mathcal{C}_{\pm} . More precisely, the following proposition holds:

PROPOSITION 3.1 *The boundary operators \mathcal{B}_{\pm} and \mathcal{C}_{\pm} satisfy the properties:*

$$\begin{aligned} \mathcal{B}_-(-\lambda) &= -\frac{\sinh(2\lambda + \eta)}{\sinh(2\lambda - \eta)} \mathcal{B}_-(\lambda), & \mathcal{C}_-(-\lambda) &= -\frac{\sinh(2\lambda + \eta)}{\sinh(2\lambda - \eta)} \mathcal{C}_-(\lambda), \\ \mathcal{B}_+(-\lambda) &= -\frac{\sinh(2\lambda - \eta)}{\sinh(2\lambda + \eta)} \mathcal{B}_+(\lambda), & \mathcal{C}_+(-\lambda) &= -\frac{\sinh(2\lambda - \eta)}{\sinh(2\lambda + \eta)} \mathcal{C}_+(\lambda). \end{aligned}$$

Proof — Such properties are simple consequences of the boundary-bulk operator decompositions following from (2.19)-(2.20). \square

Note that the proportionality factors appearing in Proposition 3.1 are not intrinsic and could in principle be removed with an appropriate choice of the normalization of the K -matrix.

This symmetry has important consequences since the operators \mathcal{B}_- or \mathcal{B}_+ (respectively \mathcal{C}_- or \mathcal{C}_+) generate the quantum space of states of the boundary XXZ model by their multiple action on the reference state $|0\rangle$ (respectively, on the dual reference state $\langle 0|$). In particular, the previous proposition naturally suggests that the solutions of the Bethe equations (2.27) are characterized by the same \mathbb{Z}_2 symmetry, which indeed can be shown from a direct study of the Bethe equations.

PROPOSITION 3.2 *Let $\{\lambda_1, \dots, \lambda_N\}$ be a solution of the system of Bethe equations (2.27), then $\{\sigma_1 \lambda_1, \dots, \sigma_N \lambda_N\}$ is still a solution for $\sigma_j = \pm 1$, $j = 1, \dots, N$.*

Proof — This follows directly from the form of the Bethe equations (2.27). \square

As in the bulk case, the operators entries of the boundary monodromy matrix can be related by some simple relations. This is the subject of the next lemma.

LEMMA 3.1 *The following relations hold:*

$$\sigma_0^x \mathcal{U}_\pm(\lambda; \xi_\pm) \sigma_0^x = -\Gamma_x \mathcal{U}_\pm(\lambda; -\xi_\pm) \Gamma_x, \quad (3.1)$$

or explicitly:

$$\mathcal{A}_\pm(\lambda; \xi_\pm) = -\Gamma_x \mathcal{D}_\pm(\lambda; -\xi_\pm) \Gamma_x, \quad \mathcal{C}_\pm(\lambda; \xi_\pm) = -\Gamma_x \mathcal{B}_\pm(\lambda; -\xi_\pm) \Gamma_x, \quad (3.2)$$

where $\Gamma_x = \bigotimes_{k=1}^M \sigma_k^x$.

Proof — These identities follow from the definitions (2.19)-(2.20) and from the bulk identity $\sigma_0^x T(\lambda) \sigma_0^x = \Gamma_x T(\lambda) \Gamma_x$. \square

The question now arises whether the state $\langle \psi_-(\{\lambda\}) |$ (2.25) (respectively $\langle \psi_+(\{\lambda\}) |$ (2.26)) is actually related to the dual state of $|\psi_-(\{\lambda\})\rangle$ (respectively $|\psi_+(\{\lambda\})\rangle$), i.e. whether the operators $\mathcal{B}_-(\lambda)$ and $\mathcal{C}_-(\lambda)$ (respectively $\mathcal{B}_+(\lambda)$ and $\mathcal{C}_+(\lambda)$) are conjugated to each other. Indeed, if the Hermitian conjugate V^\dagger of an operator $V \in \text{End}(V_0 \otimes \mathcal{H})$ is defined as

$$V^\dagger(\lambda) = [V(\lambda)]^{t_1 \dots t_M *}, \quad (3.3)$$

where $t_1 \dots t_M$ denotes the transposition on the quantum space \mathcal{H} and $*$ the complex conjugation on c -numbers, we have the following result.

PROPOSITION 3.3 *In the vicinity of the homogeneous limit of the massless model ($\eta \in i\mathbb{R}$, $\xi_k - \eta/2 \in \mathbb{R}$ and $\xi_\pm \in i\mathbb{R}$), $\mathcal{U}_\pm(\lambda)$ has the following Hermitian conjugate:*

$$\mathcal{U}_\pm^\dagger(\lambda) = -\{\mathcal{U}_\pm(-\lambda^*)\}^{t_0}. \quad (3.4)$$

An analogous result holds in the vicinity of the homogeneous limit of the massive model ($\eta \in \mathbb{R}$, $\xi_k - \eta/2 \in i\mathbb{R}$ and $\xi_\pm - iq_\pm \pi/2 \in \mathbb{R}$ with $q_\pm = 0, 1$), namely

$$\mathcal{U}_\pm^\dagger(\lambda) = (-1)^{q_\pm} \{\mathcal{U}_\pm(\lambda^*)\}^{t_0}. \quad (3.5)$$

Proof — It follows from the conjugation properties for R and K :

$$R_{0i}^\dagger(\lambda) = -R_{0i}^{t_0}(-\lambda^*), \quad K(\lambda \pm \eta/2; \xi_\pm)^* = -K(-\lambda^* \pm \eta/2; \xi_\pm),$$

in the massless case, and

$$R_{0i}^\dagger(\lambda) = R_{0i}^{t_0}(\lambda^*), \quad K(\lambda \pm \eta/2; \xi_\pm)^* = (-1)^{q_\pm} K(\lambda^* \pm \eta/2; \xi_\pm),$$

in the massive case. \square

In the next proposition, a set of formulæ are derived to express the states of the boundary XXZ model in terms of those of the periodic bulk XXZ model.

PROPOSITION 3.4 *Let $\lambda_1, \dots, \lambda_N$ be arbitrary complex numbers. Then the boundary states $|\psi_\varepsilon(\{\lambda\})\rangle$ and $\langle\psi_\varepsilon(\{\lambda\})|$, $\varepsilon = \pm$, can be expressed in terms of the bulk states as*

$$|\psi_\varepsilon(\{\lambda\})\rangle = \sum_{\sigma_1, \dots, \sigma_N = \pm} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{B}_\varepsilon}(\lambda_1, \dots, \lambda_N; \xi_\varepsilon) \prod_{j=1}^N B(\lambda_j^\sigma) |0\rangle, \quad (3.6)$$

$$\langle\psi_\varepsilon(\{\lambda\})| = \sum_{\sigma_1, \dots, \sigma_N = \pm} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_\varepsilon}(\lambda_1, \dots, \lambda_N; \xi_\varepsilon) \langle 0| \prod_{j=1}^N C(\lambda_j^\sigma), \quad (3.7)$$

where

$$\begin{aligned} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{B}_-}(\lambda_1, \dots, \lambda_N; \xi_-) &= \prod_{j=1}^N \left[-\sigma_j \gamma(\lambda_j) a(-\lambda_j^\sigma) \frac{\sinh(2\lambda_j - \eta)}{\sinh(2\lambda_j)} \right. \\ &\quad \left. \times \sinh(\lambda_j^\sigma - \xi_- + \eta/2) \right] \prod_{1 \leq r < s \leq N} \frac{\sinh(\bar{\lambda}_{rs}^\sigma + \eta)}{\sinh(\bar{\lambda}_{rs}^\sigma)}, \end{aligned} \quad (3.8)$$

$$\begin{aligned} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-) &= \prod_{j=1}^N \left[\sigma_j \gamma(\lambda_j) d(-\lambda_j^\sigma) \frac{\sinh(2\lambda_j - \eta)}{\sinh(2\lambda_j)} \right. \\ &\quad \left. \times \sinh(\lambda_j^\sigma + \xi_- - \eta/2) \right] \prod_{1 \leq r < s \leq N} \frac{\sinh(\bar{\lambda}_{rs}^\sigma - \eta)}{\sinh(\bar{\lambda}_{rs}^\sigma)}, \end{aligned} \quad (3.9)$$

$$\begin{aligned} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_+}(\lambda_1, \dots, \lambda_N; \xi_+) &= \prod_{j=1}^N \left[-\sigma_j \gamma(\lambda_j) a(-\lambda_j^\sigma) \frac{\sinh(2\lambda_j + \eta)}{\sinh(2\lambda_j)} \right. \\ &\quad \left. \times \sinh(\lambda_j^\sigma - \xi_+ + \eta/2) \right] \prod_{1 \leq r < s \leq N} \frac{\sinh(\bar{\lambda}_{rs}^\sigma + \eta)}{\sinh(\bar{\lambda}_{rs}^\sigma)}, \end{aligned} \quad (3.10)$$

$$\begin{aligned} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{B}_+}(\lambda_1, \dots, \lambda_N; \xi_+) &= \prod_{j=1}^N \left[\sigma_j \gamma(\lambda_j) d(-\lambda_j^\sigma) \frac{\sinh(2\lambda_j + \eta)}{\sinh(2\lambda_j)} \right. \\ &\quad \left. \times \sinh(\lambda_j^\sigma + \xi_+ - \eta/2) \right] \prod_{1 \leq r < s \leq N} \frac{\sinh(\bar{\lambda}_{rs}^\sigma - \eta)}{\sinh(\bar{\lambda}_{rs}^\sigma)}, \end{aligned} \quad (3.11)$$

in which we have used the notations $\lambda_j^\sigma = \sigma_j \lambda_j$ and $\bar{\lambda}_{jk}^\sigma = \sigma_j \lambda_j + \sigma_k \lambda_k$ for $j, k = 1, \dots, N$.

Proof — Let us show (3.7) and (3.9) for the state $\langle \psi_-(\{\lambda\}) |$ by induction on N , the proofs for $\langle \psi_+(\{\lambda\}) |$ and $|\psi_\pm(\{\lambda\})\rangle$ being similar.

For $N = 1$, the expression follows from the representation (A.2) of the operator \mathcal{C}_- and from the action of D on the dual reference state $\langle 0 |$.

Let us now suppose that the decomposition (3.7)-(3.9) holds for any set of complex variables $\{\lambda_1, \dots, \lambda_N\}$. The action of $\mathcal{C}_-(\lambda_{N+1})$ on the state $\langle \psi(\{\lambda_1, \dots, \lambda_N\}) |$ can be computed from (A.2) using the expression of the bulk action of $D(\lambda_{N+1})$ [43]:

$$\langle 0 | \prod_{j=1}^N C(\lambda_j) D(\lambda_{N+1}) = \sum_{k=1}^{N+1} d(\lambda_k) \frac{\prod_{j=1}^N \sinh(\lambda_{kj} + \eta)}{\prod_{\substack{j=1 \\ j \neq k}}^{N+1} \sinh \lambda_{kj}} \langle 0 | \prod_{\substack{j=1 \\ j \neq k}}^{N+1} C(\lambda_j). \quad (3.12)$$

In such a sum we can distinguish between the direct term $k = N + 1$, and the indirect terms $k < N + 1$. Let us show that each indirect term does not contribute. The indirect terms corresponding to a given $k < N + 1$ are proportional to the states $\langle 0 | \prod_{j=1, j \neq k}^N C(\lambda_j^\sigma) C(\lambda_{N+1}) C(-\lambda_{N+1})$ with coefficients:

$$\begin{aligned} \gamma(\lambda_{N+1}) \sinh \eta \frac{\sinh(2\lambda_{N+1} - \eta)}{\sinh(2\lambda_{N+1})} \sum_{\sigma_k, \sigma_{N+1} = \pm} \sigma_{N+1} d(\sigma_k \lambda_k) \frac{\sinh(\lambda_{N+1}^\sigma - \xi_- + \eta/2)}{\sinh(\lambda_k^\sigma - \lambda_{N+1}^\sigma)} \\ \times \prod_{\substack{j=1 \\ j \neq k}}^N \frac{\sinh(\lambda_{kj}^\sigma + \eta)}{\sinh(\lambda_{kj}^\sigma)} H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-). \end{aligned} \quad (3.13)$$

There we factorize the following expression:

$$\begin{aligned} \frac{\sinh(2\lambda_{N+1} - \eta)}{\sinh(2\lambda_{N+1})} \frac{\sinh(2\lambda_k - \eta)}{\sinh(2\lambda_k)} \prod_{\substack{j=1 \\ j \neq k}}^N \frac{\sinh(\lambda_k - \lambda_j^\sigma + \eta) \sinh(\lambda_k + \lambda_j^\sigma - \eta)}{\sinh(\lambda_k - \lambda_j^\sigma) \sinh(\lambda_k + \lambda_j^\sigma)} \\ \times \sinh \eta \gamma(\lambda_{N+1}) d(\lambda_k) d(-\lambda_k) \hat{H}_{k, (\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-), \end{aligned} \quad (3.14)$$

which does not depend on the values of σ_k and σ_{N+1} . Here, $\hat{H}_{k, (\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-)$ is a part of $H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-)$ which does not contain λ_k . The remaining sum in (3.13) reads as

$$\sum_{\sigma_k, \sigma_{N+1} = \pm} \sigma_k \sigma_{N+1} \frac{\sinh(\lambda_k^\sigma + \xi_- - \eta/2) \sinh(\lambda_{N+1}^\sigma - \xi_- + \eta/2)}{\sinh(\lambda_k^\sigma - \lambda_{N+1}^\sigma)}, \quad (3.15)$$

which is zero.

Thus, only the direct action of (3.12) contributes, and it generates (3.7). \square

Remark 3.1 *The above proposition implies that, for specific values of the spectral parameters, the corresponding boundary and bulk states are proportional. For example, since $d(\xi_i) = a(\xi_i - \eta) = 0$, we have,*

$$|\psi_+(\{\xi_{i_h}\})\rangle = H_1^{\mathcal{B}+}(\{\xi_{i_h}\}; \xi_+) \prod_{h=1}^N B(\xi_{i_h})|0\rangle, \quad (3.16)$$

$$\langle\psi_-(\{\xi_{i_h}\})| = H_1^{\mathcal{C}-}(\{\xi_{i_h}\}; \xi_-) \langle 0| \prod_{h=1}^N C(\xi_{i_h}), \quad (3.17)$$

$$|\psi_-(\{\xi_{i_h} - \eta\})\rangle = H_1^{\mathcal{B}-}(\{\xi_{i_h} - \eta\}; \xi_-) \prod_{h=1}^N B(\xi_{i_h} - \eta)|0\rangle, \quad (3.18)$$

$$\langle\psi_+(\{\xi_{i_h} - \eta\})| = H_1^{\mathcal{C}+}(\{\xi_{i_h} - \eta\}; \xi_+) \langle 0| \prod_{h=1}^N C(\xi_{i_h} - \eta), \quad (3.19)$$

in which $\{\xi_{i_1}, \dots, \xi_{i_N}\}$ is a subset of $\{\xi_1, \dots, \xi_M\}$, and $H_1^{\mathcal{O}\pm}(\{\lambda\}; \xi_{\pm})$, for $\mathcal{O} = \mathcal{B}, \mathcal{C}$, denotes the coefficient $H_{(1, \dots, 1)}^{\mathcal{O}\pm}(\lambda_1, \dots, \lambda_N; \xi_{\pm})$.

Note that the previous proposition, together with the bulk decompositions of the boundary operators, allows us in principle to reformulate the quantum inverse problem for the boundary XXZ in terms of the periodic bulk one. Indeed, we will use this property, in Section 5, to compute the action of a product of local operators on a boundary state.

Now, let us recall that the two expressions (2.23)-(2.24) of the boundary transfer matrix \mathcal{T} coincide as well as the Bethe equations derived using the $|\psi_-\rangle$ boundary states (2.25) or the $|\psi_+\rangle$ ones (2.26). In absence of degeneration, these observations naturally suggest that, for any solution of the boundary Bethe equations, the corresponding eigenstates $|\psi_-(\{\lambda\})\rangle$ and $|\psi_+(\{\lambda\})\rangle$ have to be proportional to each other. Indeed, this holds as shown explicitly in the next proposition.

PROPOSITION 3.5 *Let $\{\lambda_1, \dots, \lambda_N\}$ be a solution of the system of Bethe equations (2.27). Then the corresponding eigenstates generated by \mathcal{B}_+ and \mathcal{B}_- are proportional, as well as those generated by \mathcal{C}_+ and \mathcal{C}_- :*

$$\prod_{j=1}^N \mathcal{B}_+(\lambda_j)|0\rangle = \prod_{j=1}^N \frac{\sinh(\eta + 2\lambda_j)}{\sinh(\eta - 2\lambda_j)} G(\{\lambda_a\}; \xi_+, \xi_-) \prod_{j=1}^N \mathcal{B}_-(\lambda_j)|0\rangle, \quad (3.20)$$

$$\langle 0| \prod_{j=1}^N \mathcal{C}_-(\lambda_j) = \prod_{j=1}^N \frac{\sinh(\eta - 2\lambda_j)}{\sinh(\eta + 2\lambda_j)} G(\{\lambda_a\}; \xi_-, \xi_+) \langle 0| \prod_{j=1}^N \mathcal{C}_+(\lambda_j), \quad (3.21)$$

where

$$G(\{\lambda_a\}; x, y) = \prod_{j=1}^N \frac{d(\lambda_j)}{a(\lambda_j)} \frac{\sinh(\lambda_j - x + \eta/2)}{\sinh(\lambda_j + y - \eta/2)} \prod_{1 \leq r < s \leq N} \frac{\sinh(\lambda_r + \lambda_s - \eta)}{\sinh(\lambda_r + \lambda_s + \eta)}. \quad (3.22)$$

Proof — The above identities can be proved using the boundary-bulk decomposition of Proposition 3.4, by directly showing that the two ratios

$$H_{\mathcal{B}_+/\mathcal{B}_-} = (-1)^N \frac{H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{B}_+}(\lambda_1, \dots, \lambda_N; \xi_+)}{H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{B}_-}(\lambda_1, \dots, \lambda_N; \xi_-)}, \quad (3.23)$$

$$H_{\mathcal{C}_-/\mathcal{C}_+} = (-1)^N \frac{H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_-}(\lambda_1, \dots, \lambda_N; \xi_-)}{H_{(\sigma_1, \dots, \sigma_N)}^{\mathcal{C}_+}(\lambda_1, \dots, \lambda_N; \xi_+)}, \quad (3.24)$$

do not depend on $\{\sigma_1, \dots, \sigma_N\}$ and coincide respectively with

$$\prod_{j=1}^N \frac{\sinh(2\lambda_j + \eta)}{\sinh(2\lambda_j - \eta)} G(\{\lambda_a\}; \xi_+, \xi_-) \quad \text{and} \quad \prod_{j=1}^N \frac{\sinh(2\lambda_j - \eta)}{\sinh(2\lambda_j + \eta)} G(\{\lambda_a\}; \xi_-, \xi_+).$$

Let us consider for example the ratio $H_{\mathcal{B}_+/\mathcal{B}_-}$ (3.23), which reads:

$$H_{\mathcal{B}_+/\mathcal{B}_-} = \prod_{j=1}^N \frac{\sinh(2\lambda_j + \eta)}{\sinh(2\lambda_j - \eta)} \frac{d(-\lambda_j^\sigma) \sinh(\lambda_j^\sigma + \xi_+ - \eta/2)}{a(-\lambda_j^\sigma) \sinh(\lambda_j^\sigma - \xi_- + \eta/2)} \prod_{1 \leq r < s \leq N} \frac{\sinh(\bar{\lambda}_{rs}^\sigma - \eta)}{\sinh(\bar{\lambda}_{rs}^\sigma + \eta)}.$$

The action of the transformation $\sigma_a \rightarrow -\sigma_a$ on such a ratio for a given $a \in \{1, \dots, N\}$ gives:

$$\hat{H}_{a, \mathcal{B}_+/\mathcal{B}_-} \frac{\sinh(2\lambda_a + \eta)}{\sinh(2\lambda_a - \eta)} \frac{d(\lambda_a^\sigma) \sinh(\lambda_a^\sigma - \xi_+ + \eta/2)}{a(\lambda_a^\sigma) \sinh(\lambda_a^\sigma + \xi_- + \eta/2)} \prod_{\substack{s=1 \\ s \neq a}}^N \frac{\sinh(\lambda_{as}^\sigma + \eta)}{\sinh(\lambda_{as}^\sigma - \eta)}, \quad (3.25)$$

where $\hat{H}_{a, \mathcal{B}_+/\mathcal{B}_-}$ is a part of $H_{\mathcal{B}_+/\mathcal{B}_-}$ which does not contain λ_a . Proposition 3.2 now implies that $\{\lambda_1^\sigma, \dots, \lambda_N^\sigma\}$ is a solution of Bethe equations if $\{\lambda_1, \dots, \lambda_N\}$ is a solution. Therefore, applying the Bethe equation (2.27) for $j = a$, we have

$$\begin{aligned} & \frac{d(\lambda_a^\sigma)}{a(\lambda_a^\sigma)} \frac{\sinh(\lambda_a^\sigma - \xi_+ + \eta/2)}{\sinh(\lambda_a^\sigma + \xi_- - \eta/2)} \prod_{\substack{s=1 \\ s \neq a}}^N \frac{\sinh(\lambda_{as}^\sigma + \eta)}{\sinh(\lambda_{as}^\sigma - \eta)} \\ &= \frac{d(-\lambda_a^\sigma)}{a(-\lambda_a^\sigma)} \frac{\sinh(\lambda_a^\sigma + \xi_+ - \eta/2)}{\sinh(\lambda_a^\sigma - \xi_- + \eta/2)} \prod_{\substack{s=1 \\ s \neq a}}^N \frac{\sinh(\bar{\lambda}_{as}^\sigma - \eta)}{\sinh(\bar{\lambda}_{as}^\sigma + \eta)}, \end{aligned} \quad (3.26)$$

so that (3.25) coincides with the expression of $H_{\mathcal{B}_+/\mathcal{B}_-}$. \square

3.2 Description of the ground state

The Bethe equations (2.27) can be written in the logarithmic form as

$$2Mp(\lambda_j) + g(\lambda_j; \xi_+, \xi_-) + \sum_{\substack{k=1 \\ k \neq j}}^N [\theta(\lambda_{jk}) + \theta(\bar{\lambda}_{jk})] = 2\pi n_j, \quad 1 \leq j \leq N \quad (3.27)$$

where n_j are integers (with $n_j < n_{j+1}$), and where the momentum p , the scattering phase θ and the boundary contribution g are defined as

$$p(\lambda) = \frac{i}{2M} \ln \frac{d(\lambda) a(-\lambda)}{a(\lambda) d(-\lambda)}, \quad (3.28)$$

$$\theta(\lambda) = i \ln \frac{\sinh(\eta + \lambda)}{\sinh(\eta - \lambda)}, \quad (3.29)$$

$$g(\lambda; \xi_+, \xi_-) = i \ln \frac{\sinh(\lambda - \xi_+ + \eta/2) \sinh(\lambda - \xi_- + \eta/2)}{\sinh(\lambda + \xi_+ - \eta/2) \sinh(\lambda + \xi_- - \eta/2)}. \quad (3.30)$$

In the homogeneous limit, the corresponding eigenvalues of the Hamiltonian \mathcal{H} in the spin $M - N$ sector are

$$E(\{\lambda\}) = \sinh \eta \{ \coth \xi_+ + \coth \xi_- \} + 4 \sum_{j=1}^N \{ \cos p(\lambda_j) - \Delta \}. \quad (3.31)$$

In order to characterize the ground state of the half-infinite chain $M \rightarrow \infty$, one should distinguish the two domains $-1 < \Delta \leq 1$ (massless regime) and $\Delta > 1$ (massive regime), for which we set:

$$\begin{aligned} \alpha_j &= \lambda_j, \quad \zeta = i\eta > 0, \quad \xi_- = -i\tilde{\xi}_-, \quad \text{with } -\frac{\pi}{2} < \tilde{\xi}_- \leq \frac{\pi}{2}, \quad \text{for } 1 < \Delta \leq 1, \\ \alpha_j &= i\lambda_j, \quad \zeta = -\eta > 0, \quad \xi_- = -\tilde{\xi}_- + i\delta\frac{\pi}{2}, \quad \text{with } \tilde{\xi}_- \in \mathbb{R}, \quad \text{for } \Delta > 1, \end{aligned}$$

in which $\delta = 1$ for $|h_-| < \sinh \zeta$ and $\delta = 0$ otherwise. Thus, to a given set of roots $\{\lambda_j\}$ corresponds a set of variables $\{\alpha_j\}$ given by the previous change of variables. Note that two sets of Bethe roots $\{\lambda_j\}$ and $\{\sigma_j \lambda_j\}$, where $\sigma_j = \pm$, correspond to the same Bethe vector. Therefore, we consider only solutions $\{\lambda_j\}$ such that $\Re(\alpha_j) > 0$ or $\Re(\alpha_j) = 0$, $\Im(\alpha_j) < 0$.

The ground state of the half-infinite chain $M \rightarrow \infty$ has been studied in [102], [104]. It appears that the nature of the ground state rapidities depends on the value of the boundary field h_- .

In the case where $\tilde{\xi}_- < 0$ or $\tilde{\xi}_- > \zeta/2$, the ground state of the Hamiltonian (2.1) is given in both regimes by the maximum number N of roots λ_j corresponding to real (positive) α_j such that $\cos p(\lambda_j) < \Delta$. In the thermodynamic limit $M \rightarrow \infty$, these roots λ_j form a dense distribution on an interval $[0, \Lambda]$ of the real or imaginary axis. Their density

$$\rho(\lambda_j) = \lim_{M \rightarrow \infty} [M(\lambda_{j+1} - \lambda_j)]^{-1} \quad (3.32)$$

satisfies the following integral equation:

$$\rho(\lambda) + \int_0^\Lambda [K(\lambda - \mu) + K(\lambda + \mu)] \rho(\mu) d\mu = \frac{p'(\lambda)}{\pi}. \quad (3.33)$$

Here,

$$K(\lambda) = -\frac{1}{2\pi}\theta'(\lambda) = \frac{i \sinh(2\eta)}{2\pi \sinh(\lambda + \eta) \sinh(\lambda - \eta)}, \quad (3.34)$$

and $\Lambda = +\infty$ in the massless regime, while $\Lambda = -i\pi/2$ in the massive one. We may extend the definition of ρ as the solution of (3.33) on the whole interval $[-\Lambda, \Lambda]$. It is then easy to see that $\rho(-\lambda) = \rho(\lambda)$. Therefore, ρ satisfies the equation

$$\rho(\lambda) + \int_{-\Lambda}^{\Lambda} K(\lambda - \mu) \rho(\mu) d\mu = \frac{p'(\lambda)}{\pi}, \quad (3.35)$$

which means that the density of Bethe roots for the ground state of the open chain is twice the corresponding density in the periodic case.

In the case $0 < 2\tilde{\xi}_- < \zeta$, the ground state admits also a root $\tilde{\lambda}$ (corresponding to a complex $\tilde{\alpha}$) which tends to $\eta/2 - \xi_-$ with exponentially small corrections in the large M limit. In that case, the real roots density is still given by (3.35).

All the above results are valid in the homogeneous limit. However, for technical convenience, we also introduce a family of inhomogeneous densities $\rho(\lambda, \xi)$, depending on an additional parameter ξ , as solutions of the integral equation

$$\rho(\lambda, \xi) + \int_{-\Lambda}^{\Lambda} K(\lambda - \mu) \rho(\mu, \xi) d\mu = \frac{i}{\pi} t(\lambda, \xi), \quad (3.36)$$

with

$$t(\lambda, \xi) = \frac{\sinh \eta}{\sinh(\lambda - \xi) \sinh(\lambda - \xi + \eta)}. \quad (3.37)$$

It is easy to see that $\rho(-\lambda, \eta - \xi) = \rho(\lambda, \xi)$. Then the function

$$\rho_{\text{tot}}(\lambda) = \frac{1}{2M} \sum_{k=1}^M [\rho(\lambda, \xi_k) + \rho(\lambda, \eta - \xi_k)] \quad (3.38)$$

satisfies the integral equations (3.33) and (3.35) in the inhomogeneous case, and tends to the ground state density ρ in the homogeneous limit. The inhomogeneous integral equation (3.36) can be solved explicitly as

$$\rho(\lambda, \xi) = \begin{cases} \frac{i}{\zeta \sinh \frac{\pi}{\zeta}(\lambda - \xi)} & \text{in the massless regime,} \\ -\frac{1}{\pi} \prod_{n=1}^{\infty} \left(\frac{1 - q^{2n}}{1 + q^{2n}} \right)^2 \frac{\theta_2(i(\lambda - \xi), q)}{\theta_1(i(\lambda - \xi), q)}, & q = e^\eta, \text{ in the massive regime.} \end{cases}$$

Finally we would like to stress that all the functions in (3.36) are holomorphic in a symmetric strip of width η around the interval $[-\Lambda, \Lambda]$. Therefore this equation still holds at the extra root $\tilde{\lambda}$ when it exists.

4 Scalar products of boundary states

In order to compute correlation functions following the method proposed in [59], [60], it is necessary to have an explicit expression of the scalar products between a Bethe state and a general state. In the bulk case, such scalar products have been represented in the form of a determinant of usual functions in [109], [59]. The method proposed in [59] has been used in [107] to obtain a similar representation for the open XXX chain. In this section, we give the explicit expressions of the scalar products of boundary states in the XXZ case, and explain briefly how to derive them.

4.1 Partition functions

It is useful, as a starting point for the computation of scalar products, to consider the following functions:

$$\mathcal{Z}_M^{\mathcal{B}\pm}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_\pm) = \langle \bar{0} | \mathcal{B}_\pm(\lambda_M) \dots \mathcal{B}_\pm(\lambda_1) | 0 \rangle, \quad (4.1)$$

$$\mathcal{Z}_M^{\mathcal{C}\pm}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_\pm) = \langle 0 | \mathcal{C}_\pm(\lambda_M) \dots \mathcal{C}_\pm(\lambda_1) | \bar{0} \rangle, \quad (4.2)$$

where $|\bar{0}\rangle$ is the reference state with all spin down and $\langle \bar{0} |$ is its dual. Note that these functions correspond to the partition functions of the six-vertex model with domain wall boundary conditions and one reflecting end.

PROPOSITION 4.1 *The above partition functions are related to each others in the following way:*

$$\mathcal{Z}_M^{\mathcal{B}\pm}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_\pm) = (-1)^M \mathcal{Z}_M^{\mathcal{C}\pm}(\{\lambda_\alpha\}, \{\xi_k\}; -\xi_\pm), \quad (4.3)$$

$$\mathcal{Z}_M^{\mathcal{B}+}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_+) = (-1)^M \mathcal{Z}_M^{\mathcal{C}-}(\{-\lambda_\alpha\}, \{\xi_k\}; \xi_+), \quad (4.4)$$

$$\mathcal{Z}_M^{\mathcal{C}+}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_+) = (-1)^M \mathcal{Z}_M^{\mathcal{B}-}(\{-\lambda_\alpha\}, \{\xi_k\}; \xi_+). \quad (4.5)$$

Proof — As $\Gamma_x |0\rangle = |\bar{0}\rangle$ and $\langle \bar{0} | \Gamma_x = \langle 0 |$, the relations (4.3) are direct consequences of Lemma 3.1. The other two identities can be proved using the boundary-bulk decomposition of Proposition 3.4. \square

PROPOSITION 4.2 [110] *The partition function $\mathcal{Z}_M^{\mathcal{C}-}$ can be represented as the determinant*

$$\begin{aligned} \mathcal{Z}_M^{\mathcal{C}-}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_-) &= \prod_{\beta=1}^M [\gamma(\lambda_\beta) a(\lambda_\beta) a(-\lambda_\beta)] \\ &\times \frac{\prod_{\beta=1}^M \prod_{k=1}^M [\sinh(\lambda_\beta - \xi_k) \sinh(\lambda_\beta + \xi_k)]}{\prod_{\beta < \gamma} [\sinh \lambda_{\beta\gamma} \sinh \bar{\lambda}_{\beta\gamma}] \prod_{r < s} [\sinh \xi_{sr} \sinh(\bar{\xi}_{sr} - \eta)]} \det_M \mathcal{N}^{\mathcal{C}-}(\lambda_\alpha, \xi_k; \xi_-), \quad (4.6) \end{aligned}$$

where

$$\mathcal{N}_{\alpha k}^{\mathcal{C}-} = \frac{\sinh \eta \sinh(2\lambda_\alpha - \eta) \sinh(\xi_- + \xi_k - \eta/2)}{\sinh(\lambda_\alpha - \xi_k + \eta) \sinh(\lambda_\alpha + \xi_k - \eta) \sinh(\lambda_\alpha - \xi_k) \sinh(\lambda_\alpha + \xi_k)}. \quad (4.7)$$

Proof — In [110], both a set of recursion relations and the corresponding solutions were obtained.

We propose in Appendix B an alternate derivation of this representation. It is based, just as in [59], on direct calculations in the basis induced by the twist F introduced in [58]. \square

4.2 Scalar products

Let us define, for two sets of complex variables $\{\lambda_1, \dots, \lambda_N\}$ and $\{\mu_1, \dots, \mu_N\}$, the following different scalar products:

$$\mathcal{S}_N^{\varepsilon_1, \varepsilon_2}(\{\lambda\}; \{\mu\}) = \langle \psi_{\varepsilon_1}(\{\lambda\}) | \psi_{\varepsilon_2}(\{\mu\}) \rangle, \quad (4.8)$$

for $\varepsilon_1, \varepsilon_2 \in \{+, -\}$.

THEOREM 4.1 *Let $\{\lambda_1, \dots, \lambda_N\}$ be a solution of the system of Bethe equations (2.27) and $\{\mu_1, \dots, \mu_N\}$ be generic complex numbers. Then, the scalar products between the state $|\psi_+(\{\mu\})\rangle$ and the eigenstate $\langle \psi_-(\{\lambda\})|$, and between the state $\langle \psi_+(\{\mu\})|$ and the eigenstate $|\psi_-(\{\lambda\})\rangle$, are respectively given as*

$$\mathcal{S}_N^{-,+}(\{\lambda\}; \{\mu\}) = \prod_{a=1}^N [\gamma(\lambda_a) d(\lambda_a) d(-\lambda_a)] \frac{\det_N \mathcal{T}(\{\lambda\}, \{\mu\})}{\det_N \mathcal{V}(\{\lambda\}, \{\mu\})}, \quad (4.9)$$

$$\mathcal{S}_N^{+,-}(\{\mu\}; \{\lambda\}) = \prod_{a=1}^N [\gamma(\lambda_a) a(\lambda_a) a(-\lambda_a)] \frac{\det_N \mathcal{T}(\{\lambda\}, \{\mu\})}{\det_N \mathcal{V}(\{\lambda\}, \{\mu\})}, \quad (4.10)$$

where the matrices \mathcal{T} and \mathcal{V} are defined as

$$\mathcal{T}_{\alpha\beta}(\{\lambda\}, \{\mu\}) = \frac{\partial}{\partial \lambda_\alpha} \tau(\mu_\beta, \{\lambda\}) \quad (4.11)$$

$$\mathcal{V}_{\alpha\beta}(\{\lambda\}, \{\mu\}) = \frac{\sinh(2\lambda_\alpha) \sinh(2\mu_\beta - \eta)}{\sinh(2\lambda_\alpha - \eta) \sinh(\mu_\beta - \lambda_\alpha) \sinh(\mu_\beta + \lambda_\alpha)}, \quad (4.12)$$

in which $\tau(\mu_\beta, \{\lambda\})$ denotes the eigenvalue (2.31) of the transfer matrix $\mathcal{T}(\mu)$ on a Bethe eigenstate parametrized by $\{\lambda_1, \dots, \lambda_N\}$.

Proof — Let us for example consider the scalar product (4.9). This formula can be proved following the same procedure as in [59] for the bulk case. As the reference state is invariant under the action of the operator F , we can rewrite this scalar product

in the F -basis and use the explicit representations $\tilde{\mathcal{C}}_-$ and $\tilde{\mathcal{B}}_+$ given in Lemma 7.1 for the operators \mathcal{C}_- and \mathcal{B}_+ in this basis:

$$\mathcal{S}_N^{-,+}(\{\lambda\}; \{\mu\}) = \langle 0 | \prod_{a=1}^N \tilde{\mathcal{C}}_-(\lambda_a) \prod_{b=1}^N \tilde{\mathcal{B}}_+(\mu_b) | 0 \rangle. \quad (4.13)$$

The idea is then to insert, in front of each operator $\tilde{\mathcal{B}}_+$, a sum over the complete set of spin states $|i_1, \dots, i_m\rangle$, where $|i_1, \dots, i_m\rangle$ is the state with m spins down in the sites i_1, \dots, i_m and $M - m$ spins up in the other sites. We are thus led to consider intermediate functions of the form

$$\begin{aligned} G^{(m)}(\{\lambda_k\}, \mu_1, \dots, \mu_m, i_{m+1}, \dots, i_N) \\ = \langle 0 | \prod_{a=1}^N \tilde{\mathcal{C}}_-(\lambda_a) \prod_{b=1}^m \tilde{\mathcal{B}}_+(\mu_b) | i_{m+1}, \dots, i_N \rangle. \end{aligned} \quad (4.14)$$

which satisfy the following simple recursion relation:

$$\begin{aligned} G^{(m)}(\{\lambda_k\}, \mu_1, \dots, \mu_m, i_{m+1}, \dots, i_N) \\ = \sum_{j \neq i_{m+1}, \dots, i_N} \langle j, i_{m+1}, \dots, i_N | \tilde{\mathcal{B}}_+(\mu_m) | i_{m+1}, \dots, i_N \rangle \\ \times G^{(m-1)}(\{\lambda_k\}, \mu_1, \dots, \mu_{m-1}, j, i_{m+1}, \dots, i_N), \end{aligned} \quad (4.15)$$

Note that the last of this function is precisely the scalar product we want to compute,

$$G^{(N)}(\{\lambda_k\}, \mu_1, \dots, \mu_N) = \langle \psi_-(\{\lambda\}) | \psi_+(\{\mu\}) \rangle, \quad (4.16)$$

whereas the first one,

$$G^{(0)}(\{\lambda_k\}, i_1, \dots, i_N) = \langle 0 | \prod_{a=1}^N \tilde{\mathcal{C}}_-(\lambda_a) | i_1, \dots, i_N \rangle,$$

is closely related to the partition function computed in the previous section:

$$\begin{aligned} G^{(0)}(\{\lambda_k\}, i_1, \dots, i_N) = \prod_{l \neq i_1, \dots, i_N} \left\{ \prod_{\alpha=1}^N [b(\lambda_\alpha - \xi_l) b(-\lambda_\alpha - \xi_l)] \prod_{\beta=1}^N b^{-1}(\xi_{i_\beta} - \xi_l) \right\} \\ \times \mathcal{Z}_N^{\mathcal{C}_-}(\{\lambda_1, \dots, \lambda_N\}, \{\xi_{i_1}, \dots, \xi_{i_N}\}; \xi_-). \end{aligned} \quad (4.17)$$

Solving the recursion (4.15) we obtain, when particularizing the result to the case $m = N$,

$$\begin{aligned} \langle 0 | \prod_{a=1}^N \mathcal{C}_-(\lambda_a) \prod_{b=1}^N \mathcal{B}_+(\mu_b) | 0 \rangle = \frac{\sinh^N \eta \prod_{a=1}^N [\gamma(\lambda_a) d(\lambda_a) d(-\lambda_a)]}{\prod_{a>b}^N [\sinh \lambda_{ab} \sinh \bar{\lambda}_{ab} \sinh \mu_{ba} \sinh \bar{\mu}_{ba}]} \\ \times \prod_{b=1}^N \frac{\sinh(2\lambda_b - \eta) \sinh(2\mu_b + \eta)}{\sinh(2\mu_b)} \det_N H_{\alpha\beta}(\{\lambda\}, \{\mu\}), \end{aligned} \quad (4.18)$$

with

$$H_{\alpha\beta}(\{\lambda\}, \{\mu\}) = \frac{\gamma(\mu_\beta) \{y_\alpha(\mu_\beta; \{\lambda\}) - y_\alpha(-\mu_\beta; \{\lambda\})\}}{\sinh(\lambda_\alpha - \mu_\beta) \sinh(\lambda_\alpha + \mu_\beta)}. \quad (4.19)$$

This ends the proof of (4.9).

As for (4.10), it can be proved following the same procedure, provided one writes the operators \mathcal{C}_+ and \mathcal{B}_- in the \overline{F} -basis as in Lemma 7.1. \square

All the remaining scalar products can be expressed in terms of those given in Theorem 4.1. Indeed, we have the following corollary.

COROLLARY 4.1 *Let $\{\lambda_1, \dots, \lambda_N\}$ be a solution of the system of Bethe equations (2.27) and $\{\mu_1, \dots, \mu_N\}$ be generic complex numbers. Then,*

$$\mathcal{S}_N^{-,+}(\{\mu\}; \{\lambda\}) = \mathcal{S}_N^{-,+}(\{-\lambda\}; \{-\mu\}), \quad (4.20)$$

$$\mathcal{S}_N^{+,-}(\{\lambda\}; \{\mu\}) = \mathcal{S}_N^{+,-}(\{-\mu\}; \{-\lambda\}). \quad (4.21)$$

Finally, the proportionality between \pm Bethe eigenstates, given in Proposition 3.5, allows us to complete the list of scalar products where one of the boundary states is an eigenstate.

Proof — The idea is to go to the F -basis, and then to insert, between the product of the operators $\tilde{\mathcal{C}}$ and $\tilde{\mathcal{B}}$, the identity as a sum over convenient intermediate spin states, and finally to use the results of Proposition 4.1.

For example, applying this procedure to the left hand side of (4.20) in the F -basis, one obtains the relation

$$\langle 0 | \prod_{b=1}^N \mathcal{C}_-(\mu_b) \prod_{a=1}^N \mathcal{B}_+(\lambda_a) | 0 \rangle = \langle 0 | \prod_{a=1}^N \mathcal{C}_-(-\lambda_a; \xi_+) \prod_{b=1}^N \mathcal{B}_+(-\mu_b; \xi_-) | 0 \rangle, \quad (4.22)$$

which holds for any arbitrary sets of complex numbers $\{\lambda_a\}$ and $\{\mu_b\}$. The Bethe equations and the scalar product formula (4.9) being invariant under the simultaneous exchanges $\xi_+ \rightarrow \xi_-$ and $\xi_- \rightarrow \xi_+$, we obtain, under the additionnal assumption that $\{\lambda_a\}$ is a solution of the system of Bethe equations and thanks to Proposition 3.2, that the scalar product on the right hand side of (4.22) is given by (4.9) evaluated at $\{-\lambda_a\}$ and $\{-\mu_b\}$. \square

4.3 The Gaudin formula and the orthogonality of Bethe states

The scalar product formulæ derived in the previous section can be used, as in the bulk case, to compute the norm of boundary Bethe states and prove the orthogonality of eigenstates corresponding to different solutions of the Bethe equations.

COROLLARY 4.2 *Let $\{\lambda_1, \dots, \lambda_N\}$ and $\{\mu_1, \dots, \mu_N\}$ be two different solutions of the system of the Bethe equations, that is,*

$$\{\sigma_1 \lambda_1, \dots, \sigma_N \lambda_N\} \neq \{\mu_1, \dots, \mu_N\} \quad \text{for each } \sigma_j = \pm, j = 1, \dots, N. \quad (4.23)$$

Then, for $\varepsilon_1, \varepsilon_2 \in \{+, -\}$, the scalar product $\mathcal{S}_N^{\varepsilon_1, \varepsilon_2}(\{\lambda\}; \{\mu\})$ vanishes, i.e. the corresponding Bethe states $\langle \psi_{\varepsilon_1}(\{\mu\}) |$ and $| \psi_{\varepsilon_2}(\{\lambda\}) \rangle$ are orthogonal.

Proof — Let us show the orthogonality of the Bethe states corresponding to two different solutions $\{\lambda_1, \dots, \lambda_N\}$ and $\{\mu_1, \dots, \mu_N\}$ of (2.27). In such a case, the scalar products $\mathcal{S}_N^{\varepsilon_1, \varepsilon_2}(\{\lambda\}; \{\mu\})$ are proportional to each others for the different values of $\varepsilon_1, \varepsilon_2$, and the orthogonality follows from the fact that the determinant in (4.9) is equal to zero. Indeed, there exists a non-trivial vector $v(\{\lambda\}, \{\mu\})$ such that:

$$\sum_{k=1}^N H_{jk}(\{\lambda\}, \{\mu\}) v_k(\{\lambda\}, \{\mu\}) = 0, \quad \text{for any } j = 1, \dots, N. \quad (4.24)$$

Such a vector $v(\{\lambda\}, \{\mu\})$ can be constructed in the following way:

$$v_j(\{\lambda\}, \{\mu\}) = \frac{\prod_{k=1}^N \sinh(\lambda_j - \mu_k) \prod_{k=1}^N \sinh(\lambda_j + \mu_k)}{\prod_{k \neq j} \sinh \lambda_{jk} \prod_{k \neq j} \sinh \bar{\lambda}_{jk}}. \quad (4.25)$$

To check that the equations (4.24) are satisfied with the vector (4.25), we use the explicit expression for the matrix elements $H_{jk}(\{\lambda\}, \{\mu\})$ (4.19) and apply the Bethe equations for the solution $\{\mu_1, \dots, \mu_N\}$. \square

COROLLARY 4.3 *Let $\{\lambda_1, \dots, \lambda_N\}$ be a solution of the system of Bethe equations. We have*

$$\begin{aligned} \mathcal{S}_N^{-,+}(\{\lambda\}; \{\lambda\}) &= \sinh^N \eta \frac{\prod_{a=1}^N [\gamma^2(\lambda_a) d(\lambda_a) d(-\lambda_a) y_a(-\lambda_a; \{\lambda\})]}{\prod_{a \neq b}^N [\sinh \lambda_{ab} \sinh \bar{\lambda}_{ab}]} \\ &\quad \times \prod_{j=1}^N \frac{\sinh(2\lambda_j - \eta) \sinh(2\lambda_j + \eta)}{\sinh^2(2\lambda_j)} \det_N \Phi'_{jk}(\{\lambda\}). \end{aligned} \quad (4.26)$$

Here Φ' is the Gaudin matrix:

$$\Phi'_{jk}(\{\lambda\}) = \frac{\partial}{\partial \lambda_j} \log \frac{y_k(-\lambda_k; \{\lambda\})}{y_k(\lambda_k; \{\lambda\})}, \quad (4.27)$$

with $y_j(x; \{\lambda\})$ defined as in (2.29). The norm of the corresponding Bethe eigenstate follows then from Proposition 3.5 and Proposition 3.3.

4.4 Partial scalar products in the thermodynamic limit

For the computation of correlation functions, it is useful to have an expression for partial renormalized scalar products. For some partition $\alpha_+ \cup \alpha_-$ of $\llbracket 1; N \rrbracket$, we consider the sets of variables $\{\lambda_1, \dots, \lambda_N\}$ and $\{\mu_1, \dots, \mu_N\}$, with $\{\lambda\}$ solution of the system of Bethe equations (2.27), such that

$$\{\lambda\} = \{\lambda_a\}_{a \in \alpha_-} \cup \{\lambda_b\}_{b \in \alpha_+}, \quad \{\mu\} = \{\lambda_a\}_{a \in \alpha_-} \cup \{\xi_{i_b}\}_{b \in \alpha_+}, \quad (4.28)$$

in which $\{\xi_{i_b}\}_{b \in \alpha_+}$ is a subset of $\{\xi_1, \dots, \xi_M\}$. Then,

$$\begin{aligned} \frac{\mathcal{S}_N^{+,+}(\{\lambda\}; \{\mu\})}{\mathcal{S}_N^{+,+}(\{\lambda\}; \{\lambda\})} &= \prod_{b \in \alpha_+} \frac{\gamma(\lambda_b) \sinh(2\lambda_b) \sinh(2\lambda_b - \eta) \sinh(2\xi_{i_b} + \eta) \hat{y}(\xi_{i_b}; \{\lambda\})}{\gamma(\xi_{i_b}) \sinh(2\xi_{i_b}) \sinh(2\xi_{i_b} - \eta) \sinh(2\lambda_b + \eta) \hat{y}(\lambda_b; \{\lambda\})} \\ &\times \prod_{\substack{a, b \in \alpha_+ \\ a > b}} \frac{\sinh(\lambda_{ba}) \sinh(\bar{\lambda}_{ba})}{\sinh(\xi_{i_b i_a}) \sinh(\bar{\xi}_{i_b i_a})} \prod_{\substack{a \in \alpha_- \\ b \in \alpha_+}} \frac{\sinh(\lambda_{ba}) \sinh(\bar{\lambda}_{ba})}{\sinh(\xi_{i_b} - \lambda_a) \sinh(\xi_{i_b} + \lambda_a)} \frac{\det_N \mathcal{M}}{\det_N \mathcal{N}}, \end{aligned}$$

with \hat{y} given by (2.29) and

$$\begin{aligned} \mathcal{N}_{ab} &= 2M\delta_{ab} \left\{ p(\lambda_a) + \frac{1}{2M} g(\lambda_a; \xi_+, \xi_-) - \frac{\pi}{M} \sum_{k=1}^N [K(\lambda_a - \lambda_k) + K(\lambda_a + \lambda_k)] \right. \\ &\quad \left. + \frac{2\pi}{M} K(2\lambda_a) \right\} + 2\pi [K(\lambda_a - \lambda_b) - K(\lambda_a + \lambda_b)], \quad (4.29) \end{aligned}$$

$$\mathcal{M}_{ab} = \begin{cases} \mathcal{N}_{ab} & \text{if } b \in \alpha_-, \\ i[t(\lambda_a, \xi_{i_b}) - t(\lambda_a, \eta - \xi_{i_b})] & \text{if } b \in \alpha_+. \end{cases} \quad (4.30)$$

It remains to characterize the ration of the two determinants of \mathcal{M} and \mathcal{N} , which reduces to the determinant of a matrix \mathcal{S} of size $|\alpha_+|$:

$$\frac{\det_N \mathcal{M}}{\det_N \mathcal{N}} = \det_{a, b \in \alpha_+} \mathcal{S}_{ab}, \quad \text{with} \quad \mathcal{S}_{ab} = \sum_{\beta=1}^N (\mathcal{N}^{-1})_{a\beta} \mathcal{M}_{\beta b}. \quad (4.31)$$

It is actually possible, as in the bulk case, to compute explicitly \mathcal{S}_{ab} for the ground state in the thermodynamic limit.

Indeed, it is easy to see that, if λ_j corresponds to a real root α_j ,

$$\sum_{\substack{p=1 \\ \alpha_p \text{ real}}}^N \mathcal{N}_{jp} \frac{\rho(\lambda_p, \xi_k) - \rho(\lambda_p, \eta - \xi_k)}{2M\rho(\lambda_p)} \xrightarrow{M \rightarrow \infty} i[t(\lambda_j, \xi_k) - t(\lambda_j, \eta - \xi_k)]. \quad (4.32)$$

This follows from the fact that, if λ_j corresponds to a real root of the ground state, the matrix element \mathcal{N}_{jp} can be expressed as

$$\mathcal{N}_{jp} = 2M\delta_{jp} \left\{ \rho(\lambda_j) + O\left(\frac{1}{M}\right) \right\} + 2\pi [K(\lambda_j - \lambda_p) - K(\lambda_j + \lambda_p)], \quad (4.33)$$

from the symmetry property $\rho(\lambda, \mu) = \rho(-\lambda, \eta - \mu)$ of the inhomogeneous density, and from the inhomogeneous integral equation (3.36).

Therefore, if the ground state contains only real roots (i.e. in the case $\tilde{\xi}_- < 0$ or $\tilde{\xi}_- > \zeta/2$),

$$\mathcal{S}_{ab} \xrightarrow{M \rightarrow \infty} \frac{\rho(\lambda, \xi_{i_b}) - \rho(\lambda_a, \eta - \xi_{i_b})}{2M\rho(\lambda_a)}. \quad (4.34)$$

Let us now consider the ground state in the case $0 < \tilde{\xi}_- < \zeta/2$, and let $\lambda_1 = \check{\lambda}$ corresponding to the complex root (i.e. $\lambda_1 \xrightarrow{M \rightarrow \infty} \eta/2 - \xi_-$); then, there exists $\gamma > 0$ such that

$$\mathcal{N}_{1p} = g'(\check{\lambda}) \left\{ \delta_{1p} [1 + O(Me^{-\gamma M})] + O(e^{-\gamma M}) \right\}, \quad (4.35)$$

with $[g'(\check{\lambda})]^{-1} \sim i \sinh(\check{\lambda} - \xi_- + \eta/2)$ in the large M limit. Therefore, using (4.32), the inhomogeneous integral equation (3.36) at the point $\check{\lambda}$ and the estimation of $(\mathcal{N}^{-1})_{a1}$ following from (4.35), we obtain that

$$\begin{aligned} \mathcal{S}_{ab} &= (\mathcal{N}^{-1})_{a1} \mathcal{M}_{1b} + \sum_{\beta=2}^N (\mathcal{N}^{-1})_{a\beta} \mathcal{M}_{\beta b}, \\ \xrightarrow{M \rightarrow \infty} &\begin{cases} i\pi \sinh(\check{\lambda} - \xi_- + \eta/2) [\rho(\check{\lambda}, \xi_{i_b}) - \rho(\check{\lambda}, \eta - \xi_{i_b})] & \text{if } a = 1, \\ \frac{\rho(\lambda_a, \xi_{i_b}) - \rho(\lambda_a, \eta - \xi_{i_b})}{2M\rho(\lambda_a)} & \text{if } a \neq 1. \end{cases} \end{aligned} \quad (4.36)$$

5 Action of local operators on a boundary state

In order to compute correlation function, one should now determine the action of the corresponding local operators on a boundary state. As in the bulk case [59], the idea is to solve the inverse scattering problem, i.e. to express local operators in terms of the generators of the Yang-Baxter algebra.

A natural idea would be to try to express these local operators directly in terms of the generators \mathcal{A}_+ , \mathcal{B}_+ , \mathcal{C}_+ , \mathcal{D}_+ (or \mathcal{A}_- , \mathcal{B}_- , \mathcal{C}_- , \mathcal{D}_-) of the *boundary* Yang-Baxter algebra. However, although it is quite easy to reconstruct in such a way a local spin operator at the first site of the chain [106], it seems much more difficult, due to the lack of translation invariance, to obtain effective formulas on the other sites of the chain. In practice, the reconstruction proposed in [106], which involves the adjoint action of the bulk translation operators $(A + D)(\xi_k)$, is unadapted to compute correlation functions of the boundary model since eigenstates of the Hamiltonian are no more eigenstates of these translation operators.

Quite surprisingly, it is actually possible to use directly a version of the *bulk* inverse problem to compute the action of local operators on a *boundary* state. In this section, we will show how to reformulate the bulk inverse problem so as to circumvent the use of the translational invariance of the chain. Then, using Proposition 3.4, we will act with the corresponding products of bulk operators on a boundary state, obtaining a sum over some bulk states that eventually reduces to a sum over boundary states.

5.1 The bulk inverse problem revisited

Let us define a family of algebra homomorphisms $\chi_i : \mathcal{H} \rightarrow \mathcal{H}$ as

$$\chi_i : X \mapsto \widehat{R}_{i,i-1} \dots \widehat{R}_{i,1} X \widehat{R}_{1,i} \dots \widehat{R}_{i-1,i}. \quad (5.1)$$

Then, for a local operator X_i at site i (i.e. which acts non trivially only on \mathcal{H}_i), $\chi_i(X_i)$ can be expressed in terms of the bulk monodromy matrix entries as

$$\chi_i(X_i) = [a(\xi_i) d(\xi_i - \eta)]^{-1} \text{tr}_0 [T_0(\xi_i) X_0] (A + D)(\xi_i - \eta), \quad (5.2)$$

$$= [a(\xi_i) d(\xi_i - \eta)]^{-1} (A + D)(\xi_i) \text{tr}_0 [\sigma_0^y T_0^{t_0}(\xi_i - \eta) \sigma_0^y X_0]. \quad (5.3)$$

To compute the bulk correlation functions, the authors of [59], [60] used the reconstruction (5.2)², together with the fact that

$$X_i = \prod_{\alpha=1}^{i-1} (A + D)(\xi_\alpha) \chi_i(X_i) \prod_{\alpha=1}^{i-1} [(A + D)(\xi_\alpha)]^{-1}. \quad (5.4)$$

This was convenient there because the product of bulk transfer matrices merely produces a numerical factor when applied on a bulk Bethe state. As it is no longer the case when applied on a boundary Bethe state, the strategy is to simplify this product instead.

We can make the following observation:

LEMMA 5.1 *The products of the bulk monodromy matrix elements $T_{\varepsilon\varepsilon'}(\xi_i) T_{\bar{\varepsilon}\bar{\varepsilon}'}(\xi_i - \eta)$ and $T_{\varepsilon'\varepsilon}(\xi_i) T_{\bar{\varepsilon}'\bar{\varepsilon}}(\xi_i)$ vanish if $\varepsilon = \bar{\varepsilon}$.*

Proof — It follows directly from the fact that $\chi_i(E_i^{\mu'\mu}) \chi_i(E_i^{\bar{\mu}\bar{\mu}'}) = \delta_{\mu,\bar{\mu}} \chi_i(E_i^{\mu'\bar{\mu}'})$ and from the expressions (5.2), (5.3) of $\chi_i(E_i^{\mu'\mu})$, $\chi_i(E_i^{\bar{\mu}\bar{\mu}'})$ in terms of the bulk monodromy matrix, in which $E_i^{\mu\mu'}$ denotes the elementary matrix at site i with elements $(E_i^{\mu\mu'})_{ab} = \delta_{a,\mu} \delta_{b,\mu'}$. \square

Remark 5.1 *Other interesting identities may be proved in the same way. For example, from the fact that $\chi_i(E_i^{12}) \chi_i(E_i^{21}) = \chi_i(E_i^{11}) \chi_i(E_i^{11})$, one obtains that $C(\xi_i) B(\xi_i - \eta) = -A(\xi_i) D(\xi_i - \eta)$.*

This result can be generalized to a product of $2m$ operator entries of the bulk monodromy matrix:

THEOREM 5.1 *For any set of inhomogeneity parameters $\{\xi_{i_1}, \dots, \xi_{i_n}\}$, the following product of bulk operators*

$$T_{\varepsilon_{i_n} \varepsilon'_{i_n}}(\xi_{i_n}) \dots T_{\varepsilon_{i_1} \varepsilon'_{i_1}}(\xi_{i_1}) T_{\bar{\varepsilon}_{i_1} \bar{\varepsilon}'_{i_1}}(\xi_{i_1} - \eta) \dots T_{\bar{\varepsilon}_{i_n} \bar{\varepsilon}'_{i_n}}(\xi_{i_n} - \eta) \quad (5.5)$$

vanishes if, for some $k \in \{i_1, \dots, i_n\}$, $\varepsilon_k = \bar{\varepsilon}_k$.

²Note that we express here the result in a slightly different form, using that $[(A + D)(\xi_i)]^{-1} = [a(\xi_i) d(\xi_i - \eta)]^{-1} (A + D)(\xi_i - \eta)$.

Proof — It can be proved by recursion on n , the case $n = 1$ following from Lemma 5.1.

Let us suppose that the result holds for $n - 1$, and consider the product (5.5) with $\varepsilon_{i_n} = \bar{\varepsilon}_{i_n}$. Using the commutation relation given by the quadratic algebra (2.18), one can move the exterior operators (at position n) $T_{\varepsilon_{i_n} \varepsilon'_{i_n}}(\xi_{i_n})$, $T_{\bar{\varepsilon}_{i_n} \bar{\varepsilon}'_{i_n}}(\xi_{i_n} - \eta)$ through those at position $n - 1$ (evaluated respectively at $\xi_{i_{n-1}}$ and $\xi_{i_{n-1}} - \eta$). Considering all possible cases for $T_{\varepsilon_{i_n} \varepsilon'_{i_n}}(\xi_{i_n})$, $T_{\bar{\varepsilon}_{i_n} \bar{\varepsilon}'_{i_n}}(\xi_{i_n} - \eta)$ and $T_{\varepsilon_{i_{n-1}} \varepsilon'_{i_{n-1}}}(\xi_{i_{n-1}})$, $T_{\bar{\varepsilon}_{i_{n-1}} \bar{\varepsilon}'_{i_{n-1}}}(\xi_{i_{n-1}} - \eta)$, it is easy to see that the resulting product of the $2(n - 1)$ inner operators should vanish due to the recursion hypothesis. \square

This leads to the following corollary concerning the reconstruction of a product of local operators acting on successive sites of the chain:

COROLLARY 5.1 *A product of elementary matrices acting on the first m sites of the chain can be expressed as the following product of entries of the bulk monodromy matrix:*

$$E_1^{\varepsilon_1 \varepsilon'_1} \dots E_m^{\varepsilon_m \varepsilon'_m} = \prod_{i=1}^m [a(\xi_i) d(\xi_i - \eta)]^{-1} \\ \times T_{\varepsilon'_1 \varepsilon_1}(\xi_1) \dots T_{\varepsilon'_m \varepsilon_m}(\xi_m) T_{\bar{\varepsilon}_m \bar{\varepsilon}_m}(\xi_m - \eta) \dots T_{\bar{\varepsilon}_1 \bar{\varepsilon}_1}(\xi_1 - \eta) \quad (5.6)$$

with $\bar{\varepsilon}_i = \varepsilon'_i + 1 \pmod{2}$.

Proof — This is a direct consequence of the solution (5.2), (5.4) of the inverse problem, of the fact that $[(A + D)(\xi_i)]^{-1} = [a(\xi_i) d(\xi_i - \eta)]^{-1} (A + D)(\xi_i - \eta)$, and of the previous theorem. \square

5.2 Action on a bulk state

Let us now establish the action of a product of elementary matrices of the form (5.6) on an arbitrary bulk state $|\{\lambda_j\}_{1 \leq j \leq N}\rangle = \prod_{j=1}^N B(\lambda_j)|0\rangle$. We refer for example to [59] for the explicit expression, in our notations, of the action on such a state of a single operator entry of the monodromy matrix³. Let us just recall that, like in (3.12), the action of $A(\mu)$ or $D(\mu)$ produces two kinds of terms: a *direct term*, which leaves the state untouched, and *indirect terms*, resulting in new states with one λ_j replaced by μ . With this terminology, the action of operators of the form (5.6) can be computed using the following lemma:

LEMMA 5.2 *The action on a bulk state $|\{\lambda_j\}_{1 \leq j \leq N}\rangle$ of a string of operators*

$$\mathcal{O}_{\varepsilon_{i_1}, \dots, \varepsilon_{i_n}}^{\varepsilon'_{i_1}, \dots, \varepsilon'_{i_n}} = \underbrace{T_{\varepsilon'_{i_n} \varepsilon_{i_n}}(\xi_{i_n}) \dots T_{\varepsilon'_{i_1} \varepsilon_{i_1}}(\xi_{i_1})}_{(1)} \underbrace{T_{\bar{\varepsilon}_{i_1} \bar{\varepsilon}_{i_1}}(\xi_{i_1} - \eta) \dots T_{\bar{\varepsilon}_{i_n} \bar{\varepsilon}_{i_n}}(\xi_{i_n} - \eta)}_{(2)} \quad (5.7)$$

with $\bar{\varepsilon}_l = \varepsilon'_l + 1 \pmod{2}$, has the following properties.

³There the action on the left was considered, but the coefficients are the same when one considers an action on the right instead.

- The only non-zero contributions of the tails operators (2) come from
 - (i) the indirect action of all $A(\xi_l - \eta)$ operators;
 - (ii) the direct action of all $D(\xi_l - \eta)$ operators.
- In what concerns the head operators (1),
 - (iii) if $\varepsilon'_l = 1$, the action of the operator $T_{\varepsilon'_l \varepsilon_l}(\xi_l)$ (i.e. $A(\xi_l)$ or $B(\xi_l)$) does not result in any substitution of a parameter $\xi_i - \eta$;
 - (iv) if $\varepsilon'_l = 2$, the action of the operator $T_{\varepsilon'_l \varepsilon_l}(\xi_l)$ (i.e. $D(\xi_l)$ or $C(\xi_l)$) substitutes $\xi_l - \eta$ with ξ_l ; moreover, if there were others parameters $\xi_j - \eta$, $j \neq l$, in the initial state, they are still present in the resulting state.

Proof — (i) and (iii) follow from the fact that $a(\xi_l - \eta) = 0$.

In order to prove (ii), let us consider the action of some operator $D(\xi_{i_l} - \eta)$: its indirect contribution produces a state of the type $B(\xi_{i_l} - \eta) | \{\mu_j\}_{1 \leq j \leq N-1} \rangle$, for a certain set of parameters $\{\mu_j\}$. However, Theorem 5.1 guarantees that the operator product

$$T_{\varepsilon'_{i_l} \varepsilon_{i_l}}(\xi_{i_l}) \mathcal{O}_{\varepsilon'_{i_1}, \dots, \varepsilon'_{i_{l-1}}}^{\varepsilon'_{i_1}, \dots, \varepsilon'_{i_{l-1}}} B(\xi_{i_l} - \eta)$$

is zero, hence (ii).

Let us now prove (iv) by induction. If $\varepsilon'_{i_1} = 2$, then $T_{\varepsilon'_{i_1} \varepsilon_{i_1}}(\xi_{i_1})$ acts on a state of the form $B(\xi_{i_1} - \eta) | \{\mu_j\} \rangle$ for a certain set of parameters $\{\mu_j\}$, and is either equal to

- $D(\xi_{i_1})$, which acts only indirectly, and which can only replace $\xi_{i_1} - \eta$ with ξ_{i_1} ; indeed, any other replacement would produce a state of the form $B(\xi_{i_1})B(\xi_{i_1} - \eta) | \{\bar{\mu}_j\} \rangle$ (where $\{\bar{\mu}_j\}$ is a subset of $\{\mu_j\}$), which is zero according to Lemma 5.1.
- $C(\xi_{i_1})$, which gives, using Remark 5.1,

$$C(\xi_{i_1}) B(\xi_{i_1} - \eta) | \{\mu_j\} \rangle = -A(\xi_{i_1}) D(\xi_{i_1} - \eta) | \{\mu_j\} \rangle; \quad (5.8)$$

$D(\xi_{i_1} - \eta)$ acts only directly since $A(\xi_{i_1})B(\xi_{i_1} - \eta) = 0$ from Lemma 5.1, and $A(\xi_{i_1})$ cannot replace any other $\xi_j - \eta$ since $a(\xi_j - \eta) = 0$.

If (iv) is proved for all operators until position $l - 1$, then, from (i), (ii), (iii) and the induction hypothesis, $T_{\varepsilon'_{i_l} \varepsilon_{i_l}}(\xi_{i_l})$ acts on a state of the form $B(\xi_{i_l} - \eta) | \{\mu_j\} \rangle$ for a certain set of parameters $\{\mu_j\}$, and the same reasoning as for $l = 1$ applies. \square

In order to express the action of a product of elementary operators $\prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j}$ on a bulk state, let us consider the following set of indices:

$$\begin{aligned} \beta_+ &= \{j : 1 \leq j \leq m, \varepsilon_j = 1\}, \quad \text{card}(\beta_+) = s', \\ \beta_- &= \{j : 1 \leq j \leq m, \varepsilon'_j = 2\}, \quad \text{card}(\beta_-) = s. \end{aligned}$$

Since our final goal is to compute correlation functions, one considers here only products such that the total number of indices in the sets β_+ and β_- is $s + s' = m$, as otherwise the corresponding ground state average value is zero. We can thus introduce a set of indices $i_p \in \{1, \dots, m\}$ such that

$$\beta_- = \{i_p\}_{p \in \{1, \dots, s\}}, \quad \text{with } i_k < i_h \text{ for } 0 < k < h \leq s, \quad (5.9)$$

$$\beta_+ = \{i_p\}_{p \in \{s+1, \dots, m\}}, \quad \text{with } i_k > i_h \text{ for } s < k < h \leq m. \quad (5.10)$$

From Corollary 5.1 and Lemma 5.2, we obtain the following result:

PROPOSITION 5.1 *The action of a product of elementary operators on an arbitrary bulk state can be written as*

$$\prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \prod_{k=1}^N B(\lambda_k) |0\rangle = \sum_{\beta_m} \mathcal{F}_{\beta_m}(\lambda_1, \dots, \lambda_{N+m}) \prod_{\substack{k=1 \\ k \notin \beta_m}}^{N+m} B(\lambda_k) |0\rangle, \quad (5.11)$$

in which we have defined $\lambda_{N+j} := \xi_{m+1-j}$ for $j \in \{1, \dots, m\}$. In (5.11), the sums are over all the sets of m indices $\beta_m = \{b_1, \dots, b_m\}$, where the b_p are defined by

$$\begin{cases} b_p \in \{1, \dots, N\} \setminus \{b_1, \dots, b_{p-1}\} & \text{for } 0 < p \leq s, \\ b_p \in \{1, \dots, N+m+1-i_p\} \setminus \{b_1, \dots, b_{p-1}\} & \text{for } s < p \leq m, \end{cases} \quad (5.12)$$

and the coefficient \mathcal{F}_{β_m} is

$$\begin{aligned} \mathcal{F}_{\beta_m}(\{\lambda\}) &= \prod_{j=1}^m \left\{ \frac{a(\lambda_{b_j})}{a(\xi_j)} \frac{\prod_{k=1}^N \sinh(\lambda_k b_j + \eta)}{\prod_{\substack{k=1 \\ k \neq b_j}}^N \sinh(\lambda_k b_j)} \prod_{k=1}^N \frac{\sinh(\lambda_k - \xi_j)}{\sinh(\lambda_k - \xi_j + \eta)} \right\} \\ &\times \prod_{1 \leq i < j \leq m} \frac{\sinh(\lambda_{b_i} b_j)}{\sinh(\lambda_{b_i} b_j + \eta)} \prod_{p=1}^s \frac{\prod_{k=i_p+1}^m \sinh(\lambda_{b_p} - \xi_k + \eta)}{\prod_{k=i_p}^m \sinh(\lambda_{b_p} - \xi_k)} \\ &\times \prod_{p=s+1}^m \frac{\prod_{k=i_p+1}^m \sinh(\xi_k - \lambda_{b_p} + \eta)}{\prod_{\substack{k=i_p \\ k \neq N+m+1-b_p}}^m \sinh(\xi_k - \lambda_{b_p})}. \end{aligned} \quad (5.13)$$

Let us point out that, if the parameters $\lambda_1, \dots, \lambda_N$ are solutions of the bulk Bethe equations, such a result agrees with what can be obtained with the method used in [60]⁴.

⁴taking into account that we consider here an action to the right, whereas in [60] we considered an action to the left.

5.3 Action on a boundary state

We use the decomposition (3.6),(3.11) of boundary states into bulk ones in order to compute the action of a string of elementary operators on an arbitrary boundary state constructed from \mathcal{B}_+ operators. It is remarkable that we are eventually able to express explicitly the result as a linear combination of such boundary states. Indeed, using the same notations as in Proposition 5.1, we have,

PROPOSITION 5.2 *The action of a product of elementary operators on a boundary state can be written as:*

$$\prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \prod_{k=1}^N \mathcal{B}_+(\lambda_k) |0\rangle = \sum_{\beta_m} \mathcal{F}_{\beta_m}^+(\{\lambda\}) \prod_{\substack{k=1 \\ k \notin \beta_m}}^{N+m} \mathcal{B}_+(\lambda_k) |0\rangle, \quad (5.14)$$

with β_m defined as in (5.12) and the coefficient $\mathcal{F}_{\beta_m}^+$ given as

$$\begin{aligned} \mathcal{F}_{\beta_m}^+(\{\lambda\}) = & \sum_{\sigma_{\alpha_+} = \pm} \prod_{j=1}^m \frac{a(\lambda_{b_j}^\sigma)}{a(\xi_j)} \frac{H_{\sigma_{\alpha_+}}^{\mathcal{B}_+}(\{\lambda_{\alpha_+}\})}{H_1^{\mathcal{B}_+}(\{\xi_{\gamma_+}\})} \prod_{1 \leq i < j \leq m} \frac{\sinh \lambda_{b_i b_j}^\sigma}{\sinh(\lambda_{b_i b_j}^\sigma + \eta)} \\ & \times \prod_{i \in \alpha_-} \prod_{\epsilon = \pm} \left\{ \prod_{j \in \alpha_+} \frac{\sinh(\lambda_j^\sigma + \epsilon \lambda_i - \eta)}{\sinh(\lambda_j^\sigma + \epsilon \lambda_i)} \prod_{j \in \gamma_+} \frac{\sinh(\xi_j + \epsilon \lambda_i)}{\sinh(\xi_j + \epsilon \lambda_i - \eta)} \right\} \\ & \times \prod_{i \in \alpha_+} \left\{ \prod_{j \in \gamma_+} \frac{\sinh(\xi_j - \lambda_i^\sigma)}{\sinh(\xi_j - \lambda_i^\sigma - \eta)} \frac{\prod_{j \in \alpha_+} \sinh(\lambda_{j i}^\sigma + \eta)}{\prod_{j \in \alpha_+ - \{i\}} \sinh(\lambda_{j i}^\sigma)} \right\} \\ & \times \prod_{p=1}^s \frac{\prod_{k=i_p+1}^m \sinh(\lambda_{b_p}^\sigma - \xi_k + \eta)}{\prod_{k=i_p}^m \sinh(\lambda_{b_p}^\sigma - \xi_k)} \prod_{p=s+1}^m \frac{\prod_{k=i_p+1}^m \sinh(\xi_k - \lambda_{b_p}^\sigma + \eta)}{\prod_{\substack{k=i_p \\ k \neq N+m+1-b_p}}^m \sinh(\xi_k - \lambda_{b_p}^\sigma)}. \end{aligned} \quad (5.15)$$

Here, the sum is performed over all $\sigma_j \in \{+, -\}$ for $j \in \alpha_+$, we have defined $\lambda_i^\sigma := \sigma_i \lambda_i$ for $i \in \beta_m$, with $\sigma_i = 1$ if $i > N$, and

$$\begin{aligned} \alpha_+ &= \beta_m \cap \{1, \dots, N\}, & \alpha_- &= \{1, \dots, N\} \setminus \alpha_+, \\ \gamma_- &= \{N + m + 1 - j\}_{j \in \beta_m \cap \{N+1, \dots, N+m\}}, & \gamma_+ &= \{1, \dots, m\} \setminus \gamma_-. \end{aligned}$$

The function $H_\sigma^{\mathcal{B}_+}(\{\lambda\})$ is the coefficient (3.11) appearing in the boundary-bulk decomposition.

6 Elementary building blocks of correlation functions

6.1 Finite chain

It is now a matter of straightforward calculations to derive the expression of elementary building blocks of correlation functions at zero temperature. They are given as the

ground state average value of products of elementary operators of the form

$$\langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle = \frac{\langle \psi_+(\{\lambda\}) | E_1^{\varepsilon_1, \varepsilon'_1} \dots E_m^{\varepsilon_m, \varepsilon'_m} | \psi_+(\{\lambda\}) \rangle}{\langle \psi_+(\{\lambda\}) | \psi_+(\{\lambda\}) \rangle}, \quad (6.1)$$

in which $\lambda_1, \dots, \lambda_N$ denote the ground state rapidities⁵.

Using Proposition 5.2 and the partial scalar product expression of Section 4.4, we obtain for the finite chain:

PROPOSITION 6.1 *The boundary elementary building blocks can be written as*

$$\langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle = \sum_{b_1=1}^N \dots \sum_{b_s=1}^N \sum_{b_{s+1}=1}^{N+m} \dots \sum_{b_m=1}^{N+m} \frac{H_{\{b_j\}}^+(\{\lambda\})}{\prod_{1 \leq l < k \leq m} \sinh \xi_{kl} \prod_{1 \leq p \leq q \leq m} \sinh(\bar{\xi}_{pq} - \eta)}, \quad (6.2)$$

in which

$$\begin{aligned} H_{\{b_j\}}^+(\{\lambda\}) &= \sum_{\sigma_{b_j}} \frac{(-1)^{s'} \prod_{i=1}^m \sigma_{b_i} \prod_{i=1}^m \prod_{j=1}^m \sinh(\lambda_{b_i}^\sigma + \xi_j - \eta)}{\prod_{1 \leq i < j \leq m} \sinh(\lambda_{b_i b_j}^\sigma + \eta) \sinh(\bar{\lambda}_{b_i b_j}^\sigma - \eta)} \prod_{k=1}^m \frac{\sinh(\xi_k + \xi_- - \eta/2)}{\sinh(\lambda_{b_k}^\sigma + \xi_- - \eta/2)} \\ &\times \prod_{p=1}^s \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_{b_p}^\sigma - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_{b_p}^\sigma - \xi_k + \eta) \right\} \\ &\times \prod_{p=s+1}^m \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_{b_p}^\sigma - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_{b_p}^\sigma - \xi_k - \eta) \right\} \det_m \Omega. \quad (6.3) \end{aligned}$$

In this expression, the sum is performed over all $\sigma_{b_j} \in \{+, -\}$ for $b_j \leq N$, and $\sigma_{b_j} = 1$ for $b_j > N$, and the $m \times m$ matrix Ω is given in terms of the matrix \mathcal{S} of Section 4.4 as

$$\Omega_{lk} = -\delta_{N+m+1-b_l, k}, \quad \text{for } b_l > N, \quad (6.4)$$

$$\Omega_{lk} = \mathcal{S}_{b_l, k}, \quad \text{for } b_l \leq N. \quad (6.5)$$

6.2 Half-infinite chain

Let us now consider the thermodynamic limit $M \rightarrow \infty$ of this quantity.

In the case where all the roots α_j describing the ground state are real, i.e. if $\tilde{\xi}_- > \zeta/2$ or $\tilde{\xi}_- < 0$ (see Section 3.2), the sums over the indices b_j from 1 to N become, as in the bulk case, integrals over the density of the ground state. More precisely, we have to perform the replacement

$$\frac{1}{M} \sum_{b_j=1}^N \sum_{\sigma_{b_j}=\pm} \sigma_{b_j} f(\lambda_{b_j}^\sigma) \xrightarrow{N \rightarrow \infty} \int_0^\Lambda d\lambda_j \rho(\lambda_j) \sum_{\sigma_j=\pm} \sigma_j f(\lambda_j^\sigma) = \int_{-\Lambda}^\Lambda d\lambda_j f(\lambda_j) \rho(\lambda_j).$$

⁵Note that, due to Proposition 3.5, we could have also chosen to compute this average value by means of states - instead of states +.

Moreover, the sums over $b_j > N$ can be written as contour integrals thanks to the identity

$$2i\pi \operatorname{Res} \rho(\lambda, \xi) \Big|_{\lambda=\xi} = -2. \quad (6.6)$$

In the region $0 < 2\tilde{\xi}_- < \zeta$, one should also take into account the existence of the complex root. The term of the sum which corresponds to $\check{\lambda}$ can also be written as a contour integral since

$$\operatorname{Res} \left[\frac{1}{\sinh(\lambda + \xi_- - \eta/2)} \right] \Big|_{\lambda=\check{\lambda}} = 1. \quad (6.7)$$

Therefore, one obtains:

$$\begin{aligned} \langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle &= \frac{(-1)^{m-s}}{\prod_{j<i} \sinh(\xi_{ij}) \prod_{i \leq j} \sinh(\bar{\xi}_{ij} - \eta)} \\ &\times \int_{\mathcal{C}} \prod_{j=1}^s d\lambda_j \int_{\tilde{\mathcal{C}}} \prod_{j=s+1}^m d\lambda_j H_m(\{\lambda_j\}; \{\xi_k\}) \det_m [\Phi(\lambda_j, \xi_k)], \end{aligned} \quad (6.8)$$

with

$$\Phi(\lambda_j, \xi_k) = \frac{1}{2} [\rho(\lambda_j, \xi_k) - \rho(\lambda_j, \eta - \xi_k)], \quad (6.9)$$

and

$$\begin{aligned} H_m(\{\lambda_j\}; \{\xi_k\}) &= \frac{\prod_{j=1}^m \prod_{k=1}^m \sinh(\lambda_j + \xi_k - \eta)}{\prod_{1 \leq i < j \leq m} \sinh(\lambda_{ij} + \eta) \sinh(\bar{\lambda}_{ij} - \eta)} \prod_{k=1}^m \frac{\sinh(\xi_k + \xi_- - \eta/2)}{\sinh(\lambda_k + \xi_- - \eta/2)} \\ &\times \prod_{p=1}^s \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_p - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_p - \xi_k + \eta) \right\} \\ &\times \prod_{p=s+1}^m \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_p - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_p - \xi_k - \eta) \right\}. \end{aligned} \quad (6.10)$$

The contours \mathcal{C} and $\tilde{\mathcal{C}}$ depend on the boundary field. They are defined as

$$\mathcal{C} = \begin{cases} [-\Lambda, \Lambda] \cup \Gamma(\check{\lambda}) & \text{if } 0 < \tilde{\xi}_- < \zeta/2, \\ [-\Lambda, \Lambda] & \text{otherwise,} \end{cases} \quad (6.11)$$

$$\tilde{\mathcal{C}} = \mathcal{C} \cup \Gamma(\{\xi_k\}). \quad (6.12)$$

where $\Gamma(\check{\lambda})$ (respectively $\Gamma(\{\xi_k\})$) surrounds $\check{\lambda}$ (respectively ξ_1, \dots, ξ_m) with index 1, all other poles being outside.

Remark 6.1 *One can easily verify, as a consistency check for the above formula, that the reduction property*

$$\langle E_1^{\varepsilon_1, \varepsilon'_1} \dots E_m^{\varepsilon_m, \varepsilon'_m} E_{m+1}^{1,1} \rangle + \langle E_1^{\varepsilon_1, \varepsilon'_1} \dots E_m^{\varepsilon_m, \varepsilon'_m} E_{m+1}^{2,2} \rangle = \langle E_1^{\varepsilon_1, \varepsilon'_1} \dots E_m^{\varepsilon_m, \varepsilon'_m} \rangle$$

from $m+1$ sites to m sites is satisfied.

Let us finally rewrite explicitly this result in the two different regimes (massive and massless) of the XXZ model, using the fact that, in both regimes, the determinant of the matrix Φ can be calculated explicitly (the corresponding expressions are given in Appendix C).

In the massless case, one gets directly:

$$\begin{aligned} \langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle &= \frac{\prod_{a=1}^m \cosh\left(\frac{\pi}{\zeta} \xi_a\right) \prod_{k < l} \left[\sinh\left(\frac{\pi}{\zeta} \xi_{kl}\right) \sinh\left(\frac{\pi}{\zeta} \bar{\xi}_{kl}\right) \right]}{\prod_{j < i} \sinh(\xi_{ij}) \prod_{i \leq j} \sinh(\bar{\xi}_{ij} + i\zeta)} \int_{\tilde{\mathcal{C}}} \prod_{j=1}^s \left(i \frac{d\lambda_j}{\zeta} \right) \\ &\times \int_{\tilde{\mathcal{C}}} \prod_{j=s+1}^m \left(\frac{d\lambda_j}{i\zeta} \right) \prod_{a=1}^m \prod_{k=1}^m \frac{\sinh(\lambda_a + \xi_k + i\zeta)}{\sinh\left(\frac{\pi}{\zeta}(\lambda_a - \xi_k)\right) \sinh\left(\frac{\pi}{\zeta}(\lambda_a + \xi_k)\right)} \\ &\times \prod_{k < l} \frac{\sinh\left(\frac{\pi}{\zeta} \lambda_{lk}\right) \sinh\left(\frac{\pi}{\zeta} \bar{\lambda}_{lk}\right)}{\sinh(\lambda_{kl} - i\zeta) \sinh(\bar{\lambda}_{kl} + i\zeta)} \prod_{k=1}^m \frac{\sinh\left(\frac{\pi}{\zeta} \lambda_k\right) \sinh(\xi_k + i\frac{\zeta}{2} + \xi_-)}{\sinh(\lambda_k + i\frac{\zeta}{2} + \xi_-)} \\ &\times \prod_{p=1}^s \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_p - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_p - \xi_k - i\zeta) \right\} \\ &\times \prod_{p=s+1}^m \left\{ \prod_{k=1}^{i_p-1} \sinh(\lambda_p - \xi_k) \prod_{k=i_p+1}^m \sinh(\lambda_p - \xi_k + i\zeta) \right\}, \end{aligned} \quad (6.13)$$

in which $\tilde{\mathcal{C}} = \mathcal{C} \cup \Gamma(\{\xi_k\})$, with

$$\mathcal{C} = \begin{cases} \mathbb{R} & \text{for } \tilde{\xi}_- < 0 \text{ or } \tilde{\xi}_- > \zeta/2, \\ \mathbb{R} \cup \Gamma(-i(\zeta/2 + \tilde{\xi}_-)) & \text{for } 0 < \tilde{\xi}_- < \zeta/2. \end{cases} \quad (6.14)$$

In the homogeneous limit $\xi_j = -i\zeta/2$, these elementary blocks have the following form:

$$\begin{aligned}
\langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle &= (-1)^{m-s+\frac{m(m-1)}{2}} \sinh^m \xi_- \left(\frac{\pi}{\zeta} \right)^{m(m+1)} \int_{\underline{\mathcal{C}}} \prod_{j=1}^s \frac{d\lambda_j}{2\zeta} \cdot \int_{\tilde{\mathcal{C}}} \prod_{j=s+1}^m \frac{d\lambda_j}{2\zeta} \\
&\times \prod_{k<l} \frac{\sinh\left(\frac{\pi}{\zeta} \lambda_{kl}\right) \sinh\left(\frac{\pi}{\zeta} \bar{\lambda}_{kl}\right)}{\sinh(\lambda_{kl} - i\zeta) \sinh(\bar{\lambda}_{kl} + i\zeta)} \prod_{k=1}^m \frac{\sinh\left(\frac{\pi}{\zeta} \lambda_k\right)}{\sinh(\lambda_k + i\frac{\zeta}{2} + \xi_-)} \\
&\times \prod_{p=1}^s \frac{\sinh^{m+i_p-1}(\lambda_p + i\frac{\zeta}{2}) \sinh^{m-i_p}(\lambda_p - i\frac{\zeta}{2})}{\cosh^{2m}\left(\frac{\pi}{\zeta} \lambda_p\right)} \\
&\times \prod_{p=s+1}^m \frac{\sinh^{m+i_p-1}(\lambda_p + i\frac{\zeta}{2}) \sinh^{m-i_p}(\lambda_p + i\frac{3\zeta}{2})}{\cosh^{2m}\left(\frac{\pi}{\zeta} \lambda_p\right)}. \tag{6.15}
\end{aligned}$$

To obtain the explicit expression of the elementary blocks in the massive regime, one performs the change of variables $\alpha_j = i\lambda_j$, $\beta_k = i\xi_k$. Hence, using the corresponding representations for the determinants of the matrix Φ , one obtains:

$$\begin{aligned}
\langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle &= \frac{\prod_{a=1}^m [\theta_3(\beta_a) \theta_4(\beta_a)] \prod_{k<l} [\theta_1(\beta_{kl}) \theta_1(\bar{\beta}_{kl})]}{\prod_{j<i} \sin(\beta_{ij}) \prod_{i \leq j} \sin(\bar{\beta}_{ij} + i\zeta)} \\
&\times \int_{\underline{\mathcal{C}}} \prod_{j=1}^s \left(i \frac{d\alpha_j}{\pi} \right) \int_{\tilde{\mathcal{C}}} \prod_{j=s+1}^m \left(\frac{d\alpha_j}{i\pi} \right) \prod_{a=1}^m \prod_{k=1}^m \frac{\sin(\alpha_a + \beta_k + i\zeta)}{\theta_1(\alpha_a - \beta_k) \theta_1(\alpha_a + \beta_k)} \\
&\times \prod_{k<l} \frac{\theta_1(\alpha_{lk}) \theta_1(\bar{\alpha}_{lk})}{\sin(\alpha_{kl} - i\zeta) \sin(\bar{\alpha}_{kl} + i\zeta)} \prod_{k=1}^m \frac{\theta_1(\alpha_k) \theta_2(\alpha_k) \sin(\beta_k + i\frac{\zeta}{2} + i\xi_-)}{\sin(\alpha_k + i\frac{\zeta}{2} + i\xi_-)} \\
&\times \prod_{p=1}^s \left\{ \prod_{k=1}^{i_p-1} \sin(\alpha_p - \beta_k) \prod_{k=i_p+1}^m \sin(\alpha_p - \beta_k - i\zeta) \right\} \\
&\times \prod_{p=s+1}^m \left\{ \prod_{k=1}^{i_p-1} \sin(\alpha_p - \beta_k) \prod_{k=i_p+1}^m \sin(\alpha_p - \beta_k + i\zeta) \right\}, \tag{6.16}
\end{aligned}$$

in which $\theta_i(\lambda) \equiv \theta_i(\lambda, q)$, with $q = e^{-\zeta}$. The integration contours are $\tilde{\mathcal{C}} = \underline{\mathcal{C}} \cup \Gamma(\{\beta_k\})$, with

$$\underline{\mathcal{C}} = \begin{cases} [-\pi/2, \pi/2] & \text{for } \tilde{\xi}_- < 0 \text{ or } \tilde{\xi}_- > \zeta/2, \\ [-\pi/2, \pi/2] \cup \Gamma(-i(\zeta/2 + \tilde{\xi}_-)) & \text{for } 0 < \tilde{\xi}_- < \zeta/2. \end{cases} \tag{6.17}$$

In the homogenous limit $\beta_j = -i\zeta/2$, the elementary building blocks for the correlation

functions are given as

$$\begin{aligned}
\langle \prod_{j=1}^m E_j^{\varepsilon_j, \varepsilon'_j} \rangle &= 2^{m(m+1)} \sinh^m \xi_- q^{-\frac{m(m-1)}{4}} \prod_{n=1}^{\infty} [(1+q^{2n})^{2m} (1-q^{2n})^{m(3m+1)}] \\
&\times (-1)^{\frac{m(m-1)}{2}} \int_{\underline{\mathcal{C}}} \prod_{j=1}^s \left(i \frac{d\alpha_j}{2\pi} \right) \int_{\tilde{\underline{\mathcal{C}}}} \prod_{j=s+1}^m \left(\frac{d\alpha_j}{2i\pi} \right) \prod_{k<l} \frac{\theta_1(\alpha_{kl}) \theta_1(\bar{\alpha}_{kl})}{\sin(\alpha_{kl} - i\zeta) \sin(\bar{\alpha}_{kl} + i\zeta)} \\
&\times \prod_{k=1}^m \frac{\theta_1(\alpha_k) \theta_2(\alpha_k)}{\sin(\alpha_k + i\frac{\zeta}{2} + i\xi_-)} \prod_{p=1}^s \frac{\sin^{m+i_p-1}(\alpha_p + i\frac{\zeta}{2}) \sin^{m-i_p}(\alpha_p - i\frac{\zeta}{2})}{\theta_4^{2m}(\alpha_p)} \\
&\times \prod_{p=s+1}^m \frac{\sin^{m+i_p-1}(\alpha_p + i\frac{\zeta}{2}) \sin^{m-i_p}(\alpha_p + i\frac{3\zeta}{2})}{\theta_4^{2m}(\alpha_p)}. \tag{6.18}
\end{aligned}$$

Let us finally remark that all these computations can also be performed in the case of an external magnetic field along the S^z direction. In that case, the integration contours and the density function will depend, like in the bulk case, on this external magnetic field.

Acknowledgments

J.M. M., N. S. and V. T. are supported by CNRS. N. K., K. K., J.M. M. and V. T. are supported by the ANR programm GIMP ANR-05-BLAN-0029-01. N. K., G. N. and V. T. are supported by the ANR programm MIB-05 JC05-52749. N. S. is supported by the French-Russian Exchange Program, the Program of RAS Mathematical Methods of the Nonlinear Dynamics, RFBR-05-01-00498, Scientific Schools 672.2006.1. N. K and N. S. would like to thank the Theoretical Physics group of the Laboratory of Physics at ENS Lyon for hospitality, which makes this collaboration possible.

7 Appendices

A Boundary creation and annihilation operators

Using the quadratic relations (2.19)-(2.20), one can express the boundary operators $\mathcal{A}_{\pm}, \mathcal{B}_{\pm}, \mathcal{C}_{\pm}, \mathcal{D}_{\pm}$ in terms of the bulk operators. Note that it may sometimes be more convenient to rewrite the creation and annihilation boundary operators \mathcal{B}_{\pm} and \mathcal{C}_{\pm} in the form

$$\begin{aligned}
\mathcal{B}_-(\lambda) &= -\gamma(\lambda) \frac{\sinh(2\lambda - \eta)}{\sinh(2\lambda)} [B(-\lambda) A(\lambda) \sinh(\lambda + \xi_- - \eta/2) \\
&\quad + B(\lambda) A(-\lambda) \sinh(\lambda - \xi_- + \eta/2)], \tag{A.1}
\end{aligned}$$

$$\begin{aligned}
\mathcal{C}_-(\lambda) &= \gamma(\lambda) \frac{\sinh(2\lambda - \eta)}{\sinh(2\lambda)} [D(-\lambda) C(\lambda) \sinh(\lambda + \xi_- - \eta/2) \\
&\quad + D(\lambda) C(-\lambda) \sinh(\lambda - \xi_- + \eta/2)], \tag{A.2}
\end{aligned}$$

and

$$\mathcal{B}_+(\lambda) = \gamma(\lambda) \frac{\sinh(2\lambda + \eta)}{\sinh(2\lambda)} \left[B(-\lambda) D(\lambda) \sinh(\lambda - \xi_+ + \eta/2) \right. \\ \left. + B(\lambda) D(-\lambda) \sinh(\lambda + \xi_+ - \eta/2) \right], \quad (\text{A.3})$$

$$\mathcal{C}_+(\lambda) = -\gamma(\lambda) \frac{\sinh(2\lambda + \eta)}{\sinh(2\lambda)} \left[A(-\lambda) C(\lambda) \sinh(\lambda - \xi_+ + \eta/2) \right. \\ \left. + A(\lambda) C(-\lambda) \sinh(\lambda + \xi_+ - \eta/2) \right]. \quad (\text{A.4})$$

It is then convenient, for the computation of partition functions and scalar products, to express the boundary operators in the F and \overline{F} -basis. The concept of factorizing F -matrices was defined in [58], following the concept of twists introduced by Drinfel'd in the theory of Quantum Groups [111], and we refer to [58] for the explicit construction of the F and \overline{F} -matrices in the periodic XXZ spin-1/2 chain and for the representations of the bulk operators in the F and \overline{F} -basis. Using the F and \overline{F} -basis expression of the bulk operator, one obtains the following result:

LEMMA 7.1 *Let $\tilde{\mathcal{X}}_{\pm}$ denote the expressions of the boundary operators \mathcal{X}_{\pm} in the F -basis, and $\overline{\mathcal{X}}_{\pm}$ their expressions in the \overline{F} -basis. Then,*

$$\tilde{\mathcal{B}}_+(\lambda) = - \sum_{i=1}^M u(-\lambda, \xi_i | \xi_+) \sigma_i^- \otimes_{j \neq i} \begin{pmatrix} b(-\lambda - \xi_j) b(\lambda - \xi_j) & 0 \\ 0 & b^{-1}(\xi_{ji}) \end{pmatrix}_{[j]}, \quad (\text{A.5})$$

$$\tilde{\mathcal{C}}_-(\lambda) = \sum_{i=1}^M u(\lambda, \xi_i | \xi_-) \sigma_i^+ \otimes_{j \neq i} \begin{pmatrix} b(\lambda - \xi_j) b(-\lambda - \xi_j) b^{-1}(\xi_i - \xi_j) & 0 \\ 0 & 1 \end{pmatrix}_{[j]}, \quad (\text{A.6})$$

and

$$\overline{\mathcal{B}}_-(\lambda) = - \sum_{i=1}^M u(\lambda, \xi_i | -\xi_-) \sigma_i^- \otimes_{j \neq i} \begin{pmatrix} 1 & 0 \\ 0 & b(-\lambda - \xi_j) b(\lambda - \xi_j) b^{-1}(\xi_{ij}) \end{pmatrix}_{[j]}, \quad (\text{A.7})$$

$$\overline{\mathcal{C}}_+(\lambda) = \sum_{i=1}^M u(-\lambda, \xi_i | -\xi_+) \sigma_i^+ \otimes_{j \neq i} \begin{pmatrix} b^{-1}(\xi_{ji}) & 0 \\ 0 & b(\lambda - \xi_j) b(-\lambda - \xi_j) \end{pmatrix}_{[j]}, \quad (\text{A.8})$$

where

$$u(\lambda, \xi | x) = \gamma(\lambda) a(\lambda) a(-\lambda) \frac{\sinh \eta \sinh(2\lambda - \eta) \sinh(x + \xi - \eta/2)}{\sinh(\lambda - \xi + \eta) \sinh(\lambda + \xi - \eta)}. \quad (\text{A.9})$$

B Partition function

In this appendix, we propose a proof of Proposition 4.2. Similarly as in [59], this derivation is based on direct calculations in the basis induced by the twist F introduced in [58]. Indeed, in this particular basis (called F -basis), the explicit expressions of the bulk operators A , B , C , D simplify drastically. Since the boundary creation and annihilation operators are quadratic in terms of the bulk operators, they have themselves

much simpler expressions in this F -basis (see Appendix A for details). As moreover the states $\langle 0|$ and $|\bar{0}\rangle$ are respectively invariant under the left-action of F and the right-action of F^{-1} , the partition function can be directly written in the F -basis as

$$\mathcal{Z}_M^{\mathcal{C}_-}(\{\lambda_\alpha\}, \{\xi_k\}; \xi_-) = \langle 0 | \tilde{\mathcal{C}}_-(\lambda_1) \dots \tilde{\mathcal{C}}_-(\lambda_M) | \bar{0} \rangle, \quad (\text{B.10})$$

where $\tilde{\mathcal{C}}_-(\lambda) = F \mathcal{C}_-(\lambda) F^{-1}$ is the expression of $\mathcal{C}_-(\lambda)$ in the basis induced by F . Using now the expression (A.6) of the operator $\tilde{\mathcal{C}}_-(\lambda)$, one obtains a new recursion formula for the partition function, which corresponds to a development of the determinant in (4.6). Indeed, acting with $\tilde{\mathcal{C}}_-(\lambda_M)$ on the state $|\bar{0}\rangle$, one has

$$\mathcal{Z}_M^{\mathcal{C}_-}(\{\lambda_\alpha\}, \{\xi_j\}; \xi_-) = \sum_{i=1}^M u(\lambda_M, \xi_i | \xi_-) \langle 0 | \tilde{\mathcal{C}}_-(\lambda_1) \dots \tilde{\mathcal{C}}_-(\lambda_{M-1}) | \bar{i} \rangle, \quad (\text{B.11})$$

where $|\bar{i}\rangle$ is the vector with all spins down except in site i and where the expression of $u(\lambda_M, \xi_i | \xi_-)$ is given by formula (A.9). Since $(\sigma_i^+)^2 = 0$, the action of the other operators $\tilde{\mathcal{C}}_-(\lambda_\alpha)$, $1 \leq \alpha \leq M-1$, on the vector $|\bar{i}\rangle$ is diagonal on the space i , so that we obtain the following recursion formula for $\mathcal{Z}_M^{\mathcal{C}_-}$:

$$\begin{aligned} \mathcal{Z}_M^{\mathcal{C}_-}(\{\lambda_\alpha\}, \{\xi_j\}; \xi_-) &= \sum_{i=1}^M c_M(\lambda_M, \xi_i, \{\xi_j\}; \xi_-) \\ &\times \mathcal{Z}_{M-1}^{\mathcal{C}_-}(\{\lambda_\alpha\}_{\alpha \neq M}, \{\xi_j\}_{j \neq i}; \xi_-). \end{aligned} \quad (\text{B.12})$$

The coefficient of the recursion is

$$c_M(\lambda_M, \xi_i, \{\xi_j\}; \xi_-) = u(\lambda_M, \xi_i | \xi_-) \prod_{k=1}^{M-1} [b(\lambda_k - \xi_i) b(-\lambda_k - \xi_i)] \prod_{j \neq i} b^{-1}(\xi_{ji}), \quad (\text{B.13})$$

which, as a meromorphic function of λ_M , can be rewritten as

$$\begin{aligned} c_M(\lambda_M, \xi_i, \{\xi_j\}; \xi_-) &= \gamma(\lambda_M) a(\lambda_M) a(-\lambda_M) \sinh(\lambda_M - \xi_i) \sinh(\lambda_M + \xi_i) \\ &\times \prod_{\beta=1}^{M-1} \frac{\sinh(\lambda_\beta - \xi_i) \sinh(\lambda_\beta + \xi_i)}{\sinh \lambda_{M\beta} \sinh \bar{\lambda}_{M\beta}} \prod_{\substack{j=1 \\ j \neq i}}^M \frac{\sinh(\lambda_M - \xi_j) \sinh(\lambda_M + \xi_j)}{\sinh \xi_{ji} \sinh(\bar{\xi}_{ji} - \eta)} \\ &\times \left\{ \mathcal{N}_{M,i}^{\mathcal{C}_-}(\lambda_M, \xi_i; \xi_-) - \sum_{\beta=1}^{M-1} g_\beta \mathcal{N}_{\beta,i}^{\mathcal{C}_-}(\lambda_\beta, \xi_i; \xi_-) \right\}. \end{aligned} \quad (\text{B.14})$$

with

$$\begin{aligned} g_\beta &= \frac{1}{\sinh 2\lambda_\beta \sinh(2\lambda_\beta - \eta)} \left(\frac{\sinh(2\lambda_\beta + \eta)}{\sinh \bar{\lambda}_{M\beta}} + \frac{\sinh(2\lambda_\beta - \eta)}{\sinh \lambda_{M\beta}} \right) \\ &\times \frac{\prod_{k=1}^{M-1} [\sinh \lambda_{Mk} \sinh \bar{\lambda}_{Mk}]}{\prod_{\substack{k=1 \\ k \neq \beta}}^{M-1} [\sinh \lambda_{\beta k} \sinh \bar{\lambda}_{\beta k}]} \prod_{j=1}^M \frac{\sinh(\lambda_\beta - \xi_j) \sinh(\lambda_\beta + \xi_j)}{\sinh(\lambda_M - \xi_j) \sinh(\lambda_M + \xi_j)}. \end{aligned}$$

This actually corresponds to the development with respect to the last line of the determinant

$$\begin{aligned} \mathcal{Z}_M^{\mathcal{C}-}(\{\lambda_\alpha\}, \{\xi_j\}; \xi_-) &= \prod_{\beta=1}^M [\gamma(\lambda_\beta) a(\lambda_\beta) a(-\lambda_\beta)] \\ &\times \frac{\prod_{\beta=1}^M \prod_{k=1}^M [\sinh(\lambda_\beta - \xi_k) \sinh(\lambda_\beta + \xi_k)]}{\prod_{\beta < \gamma} [\sinh \lambda_{\beta\gamma} \sinh \bar{\lambda}_{\beta\gamma}] \prod_{r < s} [\sinh \xi_{sr} \sinh(\bar{\xi}_{sr} - \eta)]} \det \hat{\mathcal{N}}^{\mathcal{C}-}_M, \quad (\text{B.15}) \end{aligned}$$

where $\hat{\mathcal{N}}^{\mathcal{C}-}$ is the matrix obtained from $\mathcal{N}^{\mathcal{C}-}$ by subtracting to the last line L_M the linear combination of the other lines $\sum_{\beta=1}^{M-1} g_\beta L_\beta$. Thus, as $\mathcal{N}^{\mathcal{C}-}$ and $\hat{\mathcal{N}}^{\mathcal{C}-}$ have the same determinant, this concludes the proof.

C Determinant of the densities

In this Appendix, we give the explicit expression of the determinant of the matrix Φ involving the density function of the ground state.

In the massless case it is:

$$\begin{aligned} \det [\Phi(\lambda_j, \xi_k)] &= \left(\frac{i}{\zeta}\right)^m \prod_{a=1}^m \left[\sinh\left(\frac{\pi}{\zeta} \lambda_a\right) \cosh\left(\frac{\pi}{\zeta} \xi_a\right) \right] \\ &\times \frac{\prod_{k < l} [\sinh\left(\frac{\pi}{\zeta} \xi_{kl}\right) \sinh\left(\frac{\pi}{\zeta} \bar{\xi}_{kl}\right) \sinh\left(\frac{\pi}{\zeta} \lambda_{lk}\right) \sinh\left(\frac{\pi}{\zeta} \bar{\lambda}_{lk}\right)]}{\prod_{a=1}^m \prod_{k=1}^m [\sinh \frac{\pi}{\zeta} (\lambda_a - \xi_k) \sinh \frac{\pi}{\zeta} (\lambda_a + \xi_k)]}, \quad (\text{C.16}) \end{aligned}$$

Let us now compute the determinant of the densities in the massive case, where the density of Bethe roots can be written in terms of theta functions:

$$\rho(\lambda, \xi) = -\frac{1}{\pi} \prod_{n \geq 1} \left(\frac{1 - q^{2n}}{1 + q^{2n}} \right)^2 \frac{\theta_2(i(\lambda - \xi), q)}{\theta_1(i(\lambda - \xi), q)}, \quad (\text{C.17})$$

with $q = e^\eta = e^{-\zeta}$. We therefore have to compute the following determinant:

$$\det_m [\Phi(\lambda_j, \xi_k)] = \left(\frac{-1}{2\pi}\right)^m \prod_{n \geq 1} \left(\frac{1 - q^{2n}}{1 + q^{2n}} \right)^{2m} \det_m \left[\frac{\theta_2(\alpha_j - \beta_k)}{\theta_1(\alpha_j - \beta_k)} + \frac{\theta_2(\alpha_j + \beta_k)}{\theta_1(\alpha_j + \beta_k)} \right] \quad (\text{C.18})$$

with $\alpha_j = i\beta_j$, $\beta_k = i\xi_k$.

Let us consider $\det_m [\Phi(\lambda_j, \xi_k)]$ as a certain function f of the variable α_1 . It is an elliptic function of order $4m$ with periods π and $2i\zeta$. An irreducible set of poles is

$$\{\pm\beta_1, \dots, \pm\beta_m, \pm\beta_1 + i\zeta, \dots, \pm\beta_m + i\zeta\}, \quad (\text{C.19})$$

whereas

$$\pm\alpha_2, \dots, \pm\alpha_m, \pm\alpha_2 + i\zeta, \dots, \pm\alpha_m + i\zeta \quad (\text{C.20})$$

are zeros of f . f being an odd function, $\lambda = 0$ is also a zero and, since $f(\lambda) = -f(\lambda + i\zeta)$, so is $\lambda = i\zeta$. Up to congruence, there remain two other zeros which differ by $i\zeta$, say x_0 and $x_0 + i\zeta$. Since the sum of the zeros is congruent to the sum of the poles, x_0 is either congruent to 0 or to $\pi/2$. In fact, the only choice compatible with the periods of f is $x_0 = \pi/2$. This means that, up to a constant independent of α_1 , f can be factorized as

$$\theta_1(\alpha_1) \theta_2(\alpha_1) \frac{\prod_{i=2}^m [\theta_1(\alpha_{1i}) \theta_1(\bar{\alpha}_{1i})]}{\prod_{i=1}^m [\theta_1(\alpha_1 - \beta_i) \theta_1(\alpha_1 + \beta_i)]}. \quad (\text{C.21})$$

This argument can be easily extended to all α_j , $1 \leq j \leq m$, thanks to the antisymmetry in these variables. We can also apply a similar procedure to the variables β_k , the difference being that we now deal with an even function and that the extra zeros are $-i\zeta/2$ and $i\zeta/2 - \pi/2$. Finally we obtain

$$\det_m [\Phi(\lambda_j, \xi_k)] = \left(-\frac{1}{\pi}\right)^m \prod_{i=1}^m [\theta_1(\alpha_i) \theta_2(\alpha_i) \theta_3(\beta_i) \theta_4(\beta_i)] \times \frac{\prod_{i < j} [\theta_1(\alpha_{ij}) \theta_1(\bar{\alpha}_{ij}) \theta_1(\beta_{ji}) \theta_1(\bar{\beta}_{ji})]}{\prod_{i,j=1}^m [\theta_1(\alpha_i - \beta_j) \theta_1(\alpha_i + \beta_j)]}. \quad (\text{C.22})$$

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